10/528139 Rec'd PCT/PTO 17 MAR 2005

WO 2004/026815

New compounds for the inhibition of rotamases and use thereof

The present invention is related to new compounds and the use of said compounds as an inhibitor to rotamases and for the manufacture of medicaments.

Rotamases, also referred to as peptidyl-prolyl cis-trans isomerases (PPIases) are a family of enzymes important in protein folding, assembly and transport. They act as catalysts to promote isomerization about the peptidyl-prolyl bond, which can have profound effects on protein function.

PPIases are divided into three classes, cyclophilins, FK-506 binding proteins (FKBPs) and the Pin1/parvulin class. While cyclophilins and FKBPs are distinguished by their ability to bind immunosuppressant molecules cyclosporin and FK-506, respectively, the Pin1/parvulin class binds neither of these immunosuppressants and is structurally unrelated to the other two classes. Known members of the Pin1/parvulin class include Pins 1 – 3 (Lu et al., Nature 380:544-547, 1996), Pin-L (Campbell et al., Genomics 44:157-162, 1997), parvulin (Rahfeld et al., FEBS Letts 352:180-184, 1994), dodo (Maleszka et al., Proc Natl Acad Sci USA 93:447-451, 1996) and Ess1/Pft1 (Hanes et al., Yeast 5:55-72, 1989; and Hani et al., FEBS Letts 365:198-202, 1995).

Recent research suggests that members of the Pin1/parvulin class are essential modulators of the cell cycle, and mitosis in particular. Lu et al., Nature 380:544-547, 1996 reports that depletion of Pin1/Ess1 in yeast or human cells induces mitotic arrest followed by apoptosis, indicating that enzymes in this class serve an essential function in cell division and proliferation.

Accordingly, compounds inhibiting rotamases can serve as agents for the treatment of a variety of disorders which are characterized by an inappropriate cell proliferation including cancer and infectious diseases.

In the prior art a huge number of compounds are described which are active as inhibitors to rotamase. The respective compounds are, among others, peptide derivatives such as amino methylene-peptides which are described in European patent EP 0 610 743, or non-peptidic or non-peptidomimetic molecules.

Given the importance of rotamase there is an ongoing need in the art to provide further compounds which are suitable as inhibitors to rotamases and thus suitable to be used as a medicament for those diseases wherein a rotamase is involved in the pathological mechanism.

Accordingly, the problem underlying the present invention is to provide compounds which inhibit a rotamase. A further problem underlying the present invention is to provide new compounds for the treatment of diseases the pathophysiology of which involves an imbalanced or undesired activity of a rotamase.

In a first aspect the problem underlying the present invention is solved by a compound having the structure

$$A-[X]_{t}-Y \qquad (0)$$

wherein A is selected from the group comprising cycloalkyl, substituted cycloalkyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

$$-M_1-L_1-K-L_2-M_2-$$
, $-M_1-L_1-K-L_2-M_2-$, $-M_1-L_1-K-L_2-M_2-$, $-M_1-L_1-K-L_2-M_2-$

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wherein K is selected from the group comprising

C=T,

O, S, S(O) and $S(O_2)$,

or is absent,

with =T being selected from the group comprising

=O, =S, =N-R°, =N-CN, =N-NO₂ and =CH-NO₂.

L1 and L2 are each and independently selected from the group comprising O, S and primary amines, more particularly NR^c, NR^d; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising

 $-(CR^aR^b)n-,$

 $-(CR^fR^g)m-,$

cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl, or being individually and independent from each other absent,

wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

wherein R^c, R^d and R^e are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein R^a, R^b, R^f and R^g are independently from each other selected from the group H, OR₁₇, SR₁₈, NR₁₉R₂₀, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl,

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heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In a preferred embodiment Y is different from a peptide.

In a further embodiment A is

$$R_{1}$$
- Z_{1}
 R_{5}
 R_{3} - Z_{3}
 Z_{4} - Z_{4}
OI

In a second aspect which is actually an embodiment of the first aspect of the invention, the problem is solved by a compound which has any of the structures according to formulae (I), (III), (IV) or (V):

wherein R₁, R₂, R₃ and R₄ are each independently selected from the group comprising H, OR₆, SR₇, NR₈R₉, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein R_1 and R_2 , R_2 and R_3 , R_3 and R_4 , R_1 and R_3 , R_1 and R_4 , and R_2 and R_4 may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 or 7 members,

wherein Z_1 , Z_2 , Z_3 and Z_4 are each and independently selected from the group comprising – C(O)–, –C(S)–, –C(O)– NR_{10} -, –C(S)– NR_{11} -, –C(N–CN)– NR_{12} -, –S(O)-, –S(O)– NR_{13} -, – $S(O_2)$ – NR_{14} -, –O–, and –S–, or are each and individually absent;

R₅ is selected from the group comprising H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, substituted alkylheteroaryl and -C(O)-Q;

wherein Q is selected from the group comprising H, NHR₁₅, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, and substituted alkylheteroaryl; and

R₆, R₇, R₈, R₉, R₁₀, R₁₁, R₁₂, R₁₃, R₁₄ and R₁₅ are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

wherein K is selected from the group comprising

C=T.

O, S, S(O) and $S(O_2)$,

or is absent,

with =T being selected from the group comprising

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$$=0$$
, $=S$, $=N-R^{\circ}$, $=N-CN$, $=N-NO_2$ and $=CH-NO_2$.

L1 and L2 are each and independently selected from the group comprising O, S and primary amines, more particularly NR^c, NR^d; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising $-(CR^aR^b)n$ -, $-(CR^fR^g)m$ -, cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl,

aryl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl, or being individually and independent from each other absent,

wherein D is C_1 – C_6 alkyl, preferably straight C_1 – C_6 alkyl, C_1 – C_6 alkenyl, preferably straight C_1 – C_6 alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may individually and independently comprise from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted, more preferably by 1 or 2 substituent(s) preferably each independently selected from H, halo, OR_{16} , alkyl, and substituted alkyl,

wherein n and m are each and independently selected from each other and are each any integer from 0 to 10,

whereby if n is 2 or more, the group(s) –(CR^aR^b)– which is/are repeated, can be the same or different from any of the group(s) –(CR^aR^b)–,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

whereby if m is 2 or more, the group(s) -(CR^fR^g)- which is/are repeated, can be the same or different from any of the group(s) -(CR^fR^g)-,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

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wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

wherein

R^c, R^d and R^e are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted heterocyclyl, alkylheterocyclyl, beteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; and

R^a, R^b, R^f and R^g are independently from each other selected from the group H, OR₁₇, SR₁₈, NR₁₉R₂₀, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein E is C_1 – C_6 alkyl, preferably straight C_1 – C_6 alkyl, C_1 – C_6 alkenyl, preferably straight C_1 – C_6 alkenyl, C_1 – C_6 alkynyl, preferably straight C_1 – C_6 alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may comprise individually and independently from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted by preferably 1 or 2 substituent(s) each preferably independently selected from the group comprising H, halo, OR_{21} , alkyl, and substituted alkyl.

R₁₆, R₁₇, R₁₈, R₁₉, R₂₀ and R₂₁ are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl,

substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In an embodiment Y is different from a peptide.

In an embodiment of the first and the second aspect of the present invention the moiety A and phenol moiety, respectively forms a cyclic structure with the spacer X and/or Y.

In an embodiment of the first and the second aspect of the present invention the compound is

In a further embodiment of the first and the second aspect of the present invention the compound is selected from the group comprising

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OR₅

$$[M_1-L_1-K-L_2-M_2] \xrightarrow{t} Y$$

$$R_1-Z_1 \longrightarrow [M_1-L_1-K-L_2-M_2] \xrightarrow{t} Y$$

$$R_2-Z_2 \longrightarrow [M_1-L_1-K-L_2-M_2] \xrightarrow{t} Y$$

$$R_1-Z_1$$
 R_2-Z_2
 R_3-Z_3
 R_1-Z_1
 R_1-Z_1
 R_1-Z_1
 R_2-Z_2
 R_3-Z_3
 R_3-Z_3
 R_3-Z_3
 R_3-Z_3

$$R_1$$
- Z_1 QR_5 QR_5 QR_5 QR_5 QR_5 QR_5 QR_5 QR_5 QR_5 QR_6 QR

In an embodiment of the first and the second aspect of the present invention K is C=T.

In a further embodiment of the first and the second aspect of the present invention T is selected from the group comprising O and S.

In a preferred embodiment of the first and the second aspect of the present invention T is O.

In an alternative preferred embodiment of the first and the second aspect of the present invention T is S.

In a further alternative embodiment of the first and the second aspect of the present invention. T is selected from the group comprising N-CN, N-NO₂, CH-NO₂ and N-R^e.

In an embodiment of the first and the second aspect of the present invention, more particularly the embodiment where T is either O or S, L1 and L2 are each and independently a primary amine, preferably NR^c and/or NR^d.

In an embodiment of the first and the second aspect of the present invention n = 0 and m is any integer from 0 to 10.

In an embodiment of the first and the second aspect of the present invention R_1 and/or R_3 are selected from the group comprising halo, alkyl, substituted alkyl, heterocyclyl, substituted heterocyclyl, heterocyclyl and substituted heterocyclyl. In an even more preferred embodiment R_1 is halo.

In an embodiment of the first and the second aspect of the present invention R_5 is selected from the group comprising H and -C(O)-Q. In a preferred embodiment Q is selected from alkylheterocyclyl and substituted alkylheterocyclyl. In an even more preferred embodiment Q is selected from the group comprising N-acylated morpholino-, N-acylated piperazino- and N-acyl-derivatives.

In an embodiment of the first and the second aspect of the present invention R₆ is alkyl or substituted alkyl.

In an embodiment of the first and the second aspect of the present invention R_8 and R_9 are individually and separately selected from the group comprising H, alkyl and substituted alkyl.

In an embodiment of the first and the second aspect of the present invention n and m are individually and independently any integer from 1 to 3.

In an alternative embodiment of the first and the second aspect of the present invention n is any integer from 0 to 3 and is preferably 0 or 1.

In a further alternative embodiment of the first and the second aspect of the present invention n and m are both 0.

In an embodiment of the first and the second aspect of the present invention t is 1 or 2.

In another embodiment of the first and the second aspect of the present invention R^c and/or R^d are each and independently from each other selected from the group comprising alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

In still another embodiment of the first and the second aspect of the present invention R^a , R^b , R^f and R^g are each individually and independently from each other selected from the group comprising H, OR_{17} , SR_{18} , $NR_{19}R_{20}$, halo, alkyl and substituted alkyl.

In a preferred embodiment of the first and the second aspect of the present invention Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkylnyl and substituted branched alkynyl.

In an alternate preferred embodiment of the first and the second aspect of the present invention Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, monounsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR-CZ-NR embodiment X is

and Z is preferably selected from the group comprising O, S, N-CN, N-NO2 and CH-NO2.

In an embodiment of the NR-CZ-NR embodiment m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment wherein R₅ is H.

In an embodiment of the NR-CZ-NR embodiment n is 0, preferably R₅ being selected from the group comprising H and -C(O)-Q, more preferably m being any integer from 1 to 10. In an alternative embodiment n is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment t is 1.

In an embodiment of the first and/or second aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl and substituted branched alkynyl.

In an embodiment of the first and/or second aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide. Alternatively, Y can be absent.

In an embodiment of the NR-CZ-NR embodiment R^c and/or R^d are independently from each other selected from the group alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl,

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alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR embodiment is X is

$$-(CR^aR^b)_n-NR^c-(CR^fR^g)_m-$$

In an embodiment R^a, R^b, R^c, R^d, R^e, R^f and R^g are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, heteroaryl, substituted heteroaryl.

In an embodiment R_5 is selected from the group comprising H and -C(O)-Q. Preferably R_5 is H.

In a further embodiment m is any integer between 1 and 10. Preferably n is 0.

In a still further embodiment R_5 is selected from the group comprising H and -C(O)-Q, whereby m is any integer between 1 and 10. Preferably n is 0. In an even more preferred embodiment R_5 is H.

In a preferred embodiment of the NR embodiment X is $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$, and

wherein t is 1. Preferably, Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. Preferably R_5 is selected from the group comprising H and -C(O)-Q and even more preferably R_5 is H. In a still further preferred embodiment n is 0.

In a preferred embodiment of the NR embodiment, wherein X is $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$, and

wherein t is 1m is any integer between 1 and 10, preferably m is any integer between 2 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, and more preferably R_5 is H. Also preferably Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a preferred embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably R_5 is H and even more preferably n is 0.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR-Z embodiment X is

-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and wherein Z is selected from the group comprising C(O), C(S), S(O₂), C(O)-O, and C(O)-S.

In an embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably R_5 is H.

In an embodiment n is 0.

In a further embodiment of the NR-Z embodiment X is

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-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1. Preferably Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. More preferably R_5 is selected from the group comprising H and -C(O)-Q and even more preferably R_5 is H. In any of the latter embodiments n is 0.

In a further embodiment of the NR-Z embodiment wherein X is

-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1, m is any integer between 1 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, and more preferably R_5 is H. In an embodiment of the latter embodiments Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or wherein Y is absent. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, more preferably R_5 is H. In a particularly preferred embodiment n is 0.

In the embodiment where Y is as defined in the preceding paragraph, m is preferably any integer between 2 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)–Q and more preferably R_5 is H. Even more preferably, in any of these embodiments n is 0.

In a third aspect which is actually an embodiment of the first aspect of the invention, the problem is solved by a compound which has any of the structures according to formulae (XIV), (XV), (XVI), (XVII) or (XVIII):

$$\begin{array}{c} R_2 \cdot Z_2 \\ R_1 \cdot Z_1 \\ R_5 O \end{array} \begin{array}{c} R_2 \cdot Z_2 \\ \\ Z_4 \cdot R_4 \end{array} \begin{array}{c} XVIII \\ \\ \\ E \end{array} \qquad \text{or} \qquad \begin{array}{c} R_2 \cdot Z_2 \\ \\ \\ \\ \end{array} \begin{array}{c} XVIII \\ \\ \\ \end{array}$$

wherein R₁, R₂, R₃ and R₄ are each independently selected from the group comprising H, OR₆, SR₇, NR₈R₉, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein R₁ and R₂, R₂ and R₃, R₃ and R₄, R₁ and R₃, R₁ and R₄, and R₂ and R₄ may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 or 7 members,

wherein Z_1 , Z_2 , Z_3 and Z_4 are each and independently selected from the group comprising – C(O)–, –C(S)–, –C(O)– NR_{10} -, –C(S)– NR_{11} -, –C(N–CN)– NR_{12} -, –S(O)-, – $S(O_2)$ –, – $S(O_2)$ –, – $S(O_2)$ – NR_{14} -, –O–, and –S–, or are each and individually absent;

R₅ is selected from the group comprising H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl,

substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, substituted alkylheteroaryl and -C(O)-Q;

wherein Q is selected from the group comprising H, NHR₁₅, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, and substituted alkylheteroaryl; and

R₆, R₇, R₈, R₉, R₁₀, R₁₁, R₁₂, R₁₃, R₁₄ and R₁₅ are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

$$-M1-L1-K-L2-M2-$$
, $-M1-L1-K-L2-M2-$, $-M1-L1-K-L2-M2-$, $-M1-L1-K-L2-M2-$,

wherein K is selected from the group comprising

C=T

O, S, S(O) and $S(O_2)$,

or is absent,

with =T being selected from the group comprising

$$=$$
O, $=$ S, $=$ N $-$ R e , $=$ N $-$ CN, $=$ N $-$ NO $_{2}$ and $=$ CH $-$ NO $_{2}$,

L1 and L2 are each and independently selected from the group comprising

O, S and primary amines, more particularly NR^c, NR^d; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising -(CR^aR^b)n-,
-(CR^fR^g)m-,
cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl], or being individually and independent from each other absent,

wherein D is C_1 – C_6 alkyl, preferably straight C_1 – C_6 alkyl, C_1 – C_6 alkenyl, preferably straight C_1 – C_6 alkenyl, C_1 – C_6 alkynyl, preferably straight C_1 – C_6 alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may individually and independently comprise from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted, more preferably by 1 or 2 substituent(s) preferably each independently selected from H, halo, OR_{16} , alkyl, and substituted alkyl,

wherein n and m are each and independently selected from each other and are each any integer from 0 to 10,

whereby if n is 2 or more, the group(s) –(CR^aR^b)– which is/are repeated, can be the same or different from any of the group(s) –(CR^aR^b)–,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

whereby if m is 2 or more, the group(s) -(CR^fR^g)- which is/are repeated, can be the same or different from any of the group(s) -(CR^fR^g)-,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

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wherein

R^c, R^d and R^e are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; and

R^a, R^b, R^f and R^g are independently from each other selected from the group H, OR₁₇, SR₁₈, NR₁₉R₂₀, halo, alkyl, substituted alkyl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein E is C_1 – C_6 alkyl, preferably straight C_1 – C_6 alkyl, C_1 – C_6 alkenyl, preferably straight C_1 – C_6 alkenyl, C_1 – C_6 alkynyl, preferably straight C_1 – C_6 alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may comprise individually and independently from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted by preferably 1 or 2 substituent(s) each preferably independently selected from the group comprising H, halo, OR_{21} , alkyl, and substituted alkyl.

R₁₆, R₁₇, R₁₈, R₁₉, R₂₀ and R₂₁ are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted

heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In an embodiment Y is different from a peptide.

In an embodiment of the first and the third aspect of the present invention the moiety A and phenol moiety, respectively forms a cyclic structure with the spacer X and/or Y.

In an embodiment of the first and the third aspect of the present invention the compound is

or

In a further embodiment of the first and the third aspect of the present invention the compound is selected from the group comprising

$$R_{2}Z_{2}$$
 $R_{1}-Z_{1}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{1}-Z_{1}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{2}Z_{2}$
 $R_{3}Z_{2}$
 $R_{4}-Z_{1}$
 $R_{5}Z_{2}$
 $R_{5}Z_{2}$

In an embodiment of the first and the third aspect of the present invention K is C=T.

In a further embodiment of the first and the third aspect of the present invention T is selected from the group comprising O and S.

In a preferred embodiment of the first and the third aspect of the present invention T is O.

In an alternative preferred embodiment of the first and the third aspect of the present invention T is S.

In a further alternative embodiment of the first and the third aspect of the present invention T is selected from the group comprising N-CN, N-NO₂, CH-NO₂ and N-R^c.

In an embodiment of the first and the third aspect of the present invention, more particularly the embodiment where T is either O or S, L1 and L2 are each and independently a primary amine, preferably NR^c and/or NR^d.

In an embodiment of the first and the third aspect of the present invention n = 0 and m is any integer from 0 to 10.

In an embodiment of the first and the third aspect of the present invention R₁ and/or R₃ are selected from the group comprising halo, alkyl, substituted alkyl, heterocyclyl, substituted heterocyclyl, heterocy

In an embodiment of the first and the third aspect of the present invention R₅ is selected from the group comprising H and -C(O)-Q. In a preferred embodiment Q is selected from alkylheterocyclyl and substituted alkylheterocyclyl. In an even more preferred embodiment Q is selected from the group comprising N-acylated morpholino-, N-acylated piperazino- and N-acyl-derivatives.

In an embodiment of the first and the third aspect of the present invention R_6 is alkyl or substituted alkyl.

In an embodiment of the first and the third aspect of the present invention R₈ and R₉ are individually and separately selected from the group comprising H, alkyl and substituted alkyl.

In an embodiment of the first and the third aspect of the present invention n and m are individually and independently any integer from 1 to 3.

In an alternative embodiment of the first and the third aspect of the present invention n is any integer from 0 to 3 and is preferably 0 or 1.

In a further alternative embodiment of the first and the third aspect of the present invention n and m are both 0.

In an embodiment of the first and the third aspect of the present invention t is 1 or 2.

In another embodiment of the first and the third aspect of the present invention R^c and/or R^d are each and independently from each other selected from the group comprising alkyl,

substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

In still another embodiment of the first and the third aspect of the present invention R^a , R^b , R^f and R^g are each individually and independently from each other selected from the group comprising H, OR_{17} , SR_{18} , $NR_{19}R_{20}$, halo, alkyl and substituted alkyl.

In a preferred embodiment of the first and the third aspect of the present invention Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkylnyl and substituted branched alkynyl.

In an alternate preferred embodiment of the first and the third aspect of the present invention Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR-CZ-NR embodiment X is

and Z is preferably selected from the group comprising O, S, N-CN, N-NO2 and CH-NO2.

In an embodiment of the NR-CZ-NR embodiment m is any integer from 1 to 10.

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In an embodiment of the NR-CZ-NR embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment wherein R₅ is H.

In an embodiment of the NR-CZ-NR embodiment n is 0, preferably R₅ being selected from the group comprising H and -C(O)-Q, more preferably m being any integer from 1 to 10. In an alternative embodiment n is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment t is 1.

In an embodiment of the first and/or third aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl and substituted branched alkynyl.

In an embodiment of the first and/or third aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide. Alternatively, Y can be absent.

In an embodiment of the NR-CZ-NR embodiment R^c and/or R^d are independently from each other selected from the group alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

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In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR embodiment is X is

$$-(CR^aR^b)_n-NR^c-(CR^fR^g)_m-$$

In an embodiment R^a, R^b, R^c, R^d, R^e, R^f and R^g are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, heteroaryl, substituted heteroaryl.

In an embodiment R_5 is selected from the group comprising H and -C(O)-Q. Preferably R_5 is H.

In a further embodiment m is any integer between 1 and 10. Preferably n is 0.

In a still further embodiment R_5 is selected from the group comprising H and -C(O)-Q, whereby m is any integer between 1 and 10. Preferably n is 0. In an even more preferred embodiment R_5 is H.

In a preferred embodiment of the NR embodiment X is $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$, and

wherein t is 1. Preferably, Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. Preferably R₅ is selected from the group comprising H and -C(O)-Q and even more preferably R₅ is H. In a still further preferred embodiment n is 0.

In a preferred embodiment of the NR embodiment, wherein X is $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$, and

wherein t is 1m is any integer between 1 and 10, preferably m is any integer between 2 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, and more preferably R_5 is H. Also preferably Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a preferred embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably R_5 is H and even more preferably n is 0.

In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR-Z embodiment X is

-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and wherein Z is selected from the group comprising C(O), C(S), S(O₂), C(O)-O, and C(O)-S.

In an embodiment R_5 is selected from the group comprising H and -C(O)-Q, preferably R_5 is H.

In an embodiment n is 0.

In a further embodiment of the NR-Z embodiment X is

-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1. Preferably Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. More preferably R_5 is selected from the group comprising H and -C(O)-Q and even more preferably R_5 is H. In any of the latter embodiments n is 0.

In a further embodiment of the NR-Z embodiment wherein X is

-(CR^aR^b)_n-NR^c-Z-(CR^fR^g)_m- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1, m is any integer between 1 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, and more preferably R_5 is H. In an embodiment of the latter embodiments Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or wherein Y is absent. Preferably, R_5 is selected from the group comprising H and -C(O)-Q, more preferably R_5 is H. In a particularly preferred embodiment n is 0.

In the embodiment where Y is as defined in the preceding paragraph, m is preferably any integer between 2 and 10. Preferably, R_5 is selected from the group comprising H and -C(O)– Q and more preferably R_5 is H. Even more preferably, in any of these embodiments n is 0.

As used herein, any integer between or any integer from e.g., 0 and 10 or 0 to 10 means 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10.

In an embodiment of any aspect of the present invention Y is different from a peptide. As used herein peptide means a polymer of at least two amino acids which are linked by an amide bond. Any of the amino acids may be a natural or a non natural acid.

In a preferred embodiment of any aspect of the present invention m, n and t are independently selected from each other and are preferably any integer between 0 and 5; more preferably if n is 0, m is different from 0 and if m is 0, n is different from 0.

Also as used herein the term compound(s) according to the present invention means any compound(s) according to any aspect of the present invention. If not indicated to the contrary, any embodiment of the present invention is an embodiment of any aspect of the present invention.

R^e is selected from the group comprising H, alkyl, aryl, alkoxy, aryloxy, alkylamino and arylamino.

In an even more preferred embodiment of the inventive compound R₁, R₂, R₃ R₄ and/or R₅ have independently from each other one or more groups of the formula R^f; whereby R^f is selected from the group comprising alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, alkoxy, aryloxy, arylalkoxy, alkoxycarbonyl, aryloxycarbonyl, alkanoyl, aroyl, alkanoyloxy, aroyloxy, carbamoyl, alkanoylamino, aroylamino, alkylthio, arylthio, ureido and amine.

In a further preferred embodiment

the alkylthio group is derivatized, preferably the sulfur atom of the alkylthio group is oxidized to a sulfoxide or sulfone;

the arylthio group is derivatized, preferably the sulfur atom of the arylthio group is oxidized to a sulfoxide or sulfone,

the ureido group is derivatized, preferably the nitrogen atom of the ureido group is independently mono- or di-substituted, more preferably the substitution is selected from the group comprising alkyl, aryl, heterocyclyl, heteroaryl, alkoxycarbonylamino,

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aryloxycarbonylamino, alkylcarbamoyloxy, arylcarbamoyloxy, alkylsulfonylamino, arylsulfonylamino, alkylaminosulfonyl, and arylaminosulfonyl; and/or

the amino group is derivatized, preferably the nitrogen atom is independently mono- or disubstituted by alkly, aryl, heterocyclyl, heteroalyl, halogen, hydroxy, oxo, carboxy, cyano, nitro, amidino and guanidino.

In a still more preferred embodiment R^f is further substituted by one ore more groups R^g, whereby R^g is selected from the group comprising alkyl, cycloalkyl, aryl, arylalkyl, alkoxy, aryloxy, arylalkoxy, alkanoyl, aroyl, amino, halogen, hydroxy, oxo, carboxy, cyano, nitro, amidino and guanidino.

Particularly preferred compounds according to the present invention are the compounds specified in the following table 1:

				S Ale sets		
	Structure	Chemical name	Formula	Synmesis methods	MolWeight	MS data
_		3-[3-(5-Chloro-2-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	C12H15CIN2O4	4	286.71	286.9
7	5_0 E_0 E_0	1-(5-Chloro-2-hydroxy-phenyl)-3- pentyl-urea	C12H17CIN2O2	¥	256.73	256.9
m	12 5 5 5	1-Benzyl-3-(5-chloro-2-hydroxy- phenyl)-urea	C14H13CIN2O2	∢	276.72	276.9
4	TZ TZ 5—————————————————————————————————	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	C15H15CIN2O2	∢	290.74	290.9
ν,	12 5 	1-(5-Chioro-2-hydroxy-phenyl)-3- phenethyl-urea	C15H15CIN2O2	<	290.75	291.2

1-(5-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea (1,1,3,3-tetramethyl-butyl)-urea 1-tert-Butyl-3-(5-chloro-2-hydroxy-phenyl)-3- hydroxy-phenyl)-urea 1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea 1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-beazyl)-urea	A 298.81 299.4	A 242.70 243.0	A 282.77 283.1	A 344.72 345.0	
	6	ro-2-	phenyl)-3-	froxy-phenyl)-3- -benzyl)-urea	
	1-(5-Chloro-2-hydi	IZ >=0	\bigcirc	H 1-(5-Chloro-2-hyd (4-trifluoromethyl-	TZ

		т		
297.7	331.0	269.1	346.9	. 287.9
297.14	330.69	268.74	346.69	287.70
V	¥	¥	¥	4
C13H10C1ZNZO2	C14H10CIF3N2O2	C13H17CIN2O2	C14H10CIF3N2O3	C14H10CIN3O2
1-(5-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-wea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea
5	HA DO TO	12 0 12 5	HO IN	\$ 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
=	12	13	14	15

			т	
306.9	276.9	292.9	290.9	. 353.2
306.70	276.72	292.72	290.75	352.77
∢	A	Ą	· V	¥
C14H11CIN2O4	C14H13GIN2O2	C14H13CIN2O3	C15H15CIN2O2	C16H17CIN2O5
1-Benzo[1,3]dioxol-5-yl-3-(5- chloro-2-hydroxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- o-tolyl-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea
		IN TO TO	TZ TZ TZ	OH OHO OME
91	17	81	19	20

313.1	321.4	354.9	263.2	321.9
312.75	320.82	354.79	262.70	321.16
Ą	∢	. ∢	٧	Ą
C17H13CIN2O2	C17H21CIN2O2	C19H15CIN2O3	C13H11CIN2O2	C12H14Cl2N2O4
1-(5-Chloro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(5-chloro-2- hydroxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- phenyl-urea	3-[3-(3,5-Dichloro-2-hydroxy-phenyl)-ureido]-propionic acid ethyl ester
IN TO	5—————————————————————————————————————	1Z 0 1Z 0	1Z 0 1Z 0	TIN O
21	z	23	42	22

56	5 5	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-pentyl-urea	C12H16CI2N2O2	₹	291.17	292.0
27	12 5 5 5	1-Benzyl-3-(3,5-dichloro-2- hydroxy-phenyl)-urea	C14H12Cl2N2O2	¥	311.16	312.0
78	2 IZ 0 IZ 0	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	C15H14Cl2N2O2	V	325.19	325.9
59	TIN TO TIN TO TO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenethyl-urea	C15H14Cl2N2O2	¥	325.19	325.9
30	N N D	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	C15H22CI2N2O2	¥	333.25	334.0

				
277.8	318.1	379.8	366.9	331.9
277.15	317.21	379.16	366.03	331.58
∢ .	У	A .	¥	∢
C11H14Cl2N2O2	C14H18Cl2N2O2	C15H11Cl2F3N2O2	C13H8Cl4N2O2	C13H9Cl3N2O2
1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea
2 IZ 0 IZ 0	12 5 5	IN O	2 TZ 0 TZ 0	
31	32	33	34	35

365.9	304.0	381.8	322.9	. 341.7
365.13	303.18	381.13	322.15	341.15
Ą	Ą	₩	¥	¥
C14H9Cl2F3N2O2	C13H16Cl2N2O2	C14H9Cl2F3N2O3	C14H9Cl2N3O2	C14H10Cl2N2O4
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5- dichloro-2-hydroxy-phenyl)-urea
12 0 12 0 13 0 15 0	TZ TZ	D IN	12 0 12 0 12 0	TZ O
36	37	38	39	40

311.8	327.5	325.6	387.6	. 347.6
311.16	327.16	325.19	387.21	347.20
∢	¥	ď	. ♥	¥
C14H12CIZNZO2	C14H12Cl2N2O3	C15H14Cl2N2O2	C16H17Cl2N2O5	C17H12Cl2N2O2
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-o-tolyl-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	1-(3,5-Dichloro-2-bydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3,4,5-trimethoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea
TZ O TZ	D IN	2 IZ TO	CI C	TZ TO TO
41	42	43	4	45

	Z		 	• • • • •	
355.7	389.6	297.7	286.9	. 256.9	276.9
355.26	389.23	297.14	286.71	256.73	276.72
∀	A	∢	A	Ą	¥
C17H20C12N2O2	C19H14Cl2N2O3	C13H10Cl2N2O2	C12H15CIN2O4	C12H17CIN2O2	C14H13CIN2O2
1-Adamantan-1-yl-3-(3,5-dichloro- 2-hydroxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenyl-urea	3-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(3-Chloro-2-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-chloro-2-hydroxy- phenyl)-urea
5 5 5	2 12 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	5 12 5 5		D IN DO	TN O
46	47	48	49	20	51

					T	
290.9	291.2	299.4	243.0	283.1	. 345.0	331.9
290.74	290.75	298.81	242.70	282.77	344.72	331.59
V	¥	A	Ą	4	∀	∢
C15H15CIN2O2	CISHISCIN202	CISH23CIN2O2	C11H15CINZO2	C14H19CIN2O2	C15H12CIF3N2O2	C13H9Cl3N2O2
1-(3-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- phenethyl-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3-chloro-2- hydroxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea
E S	E S S S S S S S S S S S S S S S S S S S	TZ O TZ	12 0 12 0 12 0	IZ TZ TZ	D CF3	5 12 5 5
52	53	54	55	56	57	88

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297.7	331.0	269.1	346.9	287.9	. 306.9	276.9
297.14	330.69	268.74	346.69	287.70	306.70	276.72
Ą	∢	Ą	ď	∢ `	A	¥
C13H10CIZNZO2	C14H10CIF3N2O2	C13H17CIN2O2	C14H10CIF3N2O3	C14H10CIN3O2	C14H11CIN2O4	C14H13CIN2O2
1-(3-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3- chloro-2-hydroxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- o-tolyl-urea
D IZ D	E S S S S S S S S S S S S S S S S S S S	IZ O IZ O	P N N N N N N N N N N N N N N N N N N N	H. H. D.	S N N N N N N N N N N N N N N N N N N N	IN TO THE PERSON
59	09	61	79	8	2	53

292.9	290.9	353.2	313.1	321.4	354.9
292.72	290.75	352.77	312.75	320.82	354.79
¥	A	¥	. ∢	<b>∢</b>	V
C14H13CIN2O3	C15H15CIN2O2	C16H17CIN2O5	C17H13CIN2O2	C17H21CIN2O2	C19H15CIN2O3
1-(3-Chloro-2-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-wea	1-(3-Chloro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3-chloro-2- hydroxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea
OH OH OH	TZ O	CI OMe OMe	P D IN D	2 - Z	E S
99	19	89	69	02	71

						<del></del>
263.2	270.6	240.5	260.8	274.9	274.6	282.9
262.70	270.26	240.27	260.26	274.29	274.29	282.35
A	Ą	¥	Ą	¥	<b>V</b>	. ✓
C13H11CIN2O2	C12H15FN2O4	C12H17FN2O2	C14H13FN2O2	C15H15FN2O2	C15H15FN2O2	C15H23FN2O2
1-(3-Chloro-2-hydroxy-phenyl)-3- phenyl-urea	3-[3-(3-Fluoro-2-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(3-Fluoro-2-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-fluoro-2-hydroxy- phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenethyl-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea
\$ IZ = 0	P N N	E S	F	TZ O	E S	TZ O
72	73	74	75	92	77	78

226.5	266.7	328.4	315.5	281.1	314.6
226.25	266.31	328.26	315.13	280.68	314.24
A	A	ď	<b>4</b>	¥	A
C11H15FN2O2	C14H19FN2O2	C15H12F4N2O2	C13H9C12FN2O2	C13H10CIFN2O2	C14H10F4N2O2
1-tert-Butyl-3-(3-fluoro-2- hydroxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea
HN HO	IZ FO	P H N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N	HZ HZ	HO HO
79	08	81	83	83	28

977	5.5	1.4	290.7	260.5	276.5	274.7
252.6	330.5	271.4	29	56	. 27	
252.28	330.23	271.25	290.25	260.26	276.26	274.29
¥	¥	¥	<b>V</b>	A	٧	₩
C13H17FN2O2	C14H10FF3N2O3	C14H10FFN3O3	C14H11FN2O4	C14H13FN2O2	C14H13FN2O3	C15H15FN2O2
1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexyl-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3- fluoro-2-hydroxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- o-tolyl-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea
E O	HO NI	EN SO	IN SO		H N N O N O N O N O N O N O N O N O N O	P P P P P P P P P P P P P P P P P P P
8	98	8.2	88	68	8	91

8	F H H H OMe	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	C16H17FN2O5	∢	336.31	336.6
93	TZ O	1-(3-Fluoro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	C17H13FN2O2	٧	296.3	296.6
24	₹ 5 1	1-Adamantan-1-yl-3-(3-fluoro-2- hydroxy-phenyl)-urea	C17H21FN2O2	∢ .	304.36	304.6
95	12 - S	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	C19H15FN2O3	<b>V</b>	338.33	338.6
96	TZ TZ TÖ	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenyl-urea	C13H11FN2O2	A	246.24	246.5
97	D D D D D D D D D D D D D D D D D D D	3-[3-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-ureido]-propionic acid ethyl ester	C13H16Cl2N2O4	<b>V</b>	335.19	335.9

305.9	325.5	339.9	339.4	347.4
305.20	325.19	339.22	339.22	347.28
Ą	<b>∢</b>	<b>V</b>	¥	A
C13H18CI2N2O2	C15H14Cl2N2O2	C16H16CI2N2O2	C16H16Cl2N2O2	C16H24Cl2N2O2
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-pentyl-urea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2-methyl- benzyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenethyl-urea	1-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-3-(1,1,3,3-terramethyl-butyl)-urea
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	TIN O	TN O	TZ TO TZ	E TO
86	66	100	101	102

103	IZ TO IZ TO TO TO	1-tert-Butyl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-urea	C12H16Cl2N2O2	A	291.18	291.2
104	IZ TO TO TO TO TO TO TO TO TO TO TO TO TO	1-Cyclohexylmethyl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-urea	C15H20C12N2O2	¥	331.24	332.1
105	TX O TX	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-benzyl)-urea	C16H13ClZF3N2O2	∢ .	393.19	393.8
106	D D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,5-dichloro- phenyl)-urea	C14H10Cl4N2O2	∢	380.06	380.2
107	TIN O TIN TO	1-(4-Chloro-phenyl)-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea	C14H11Cl3N2O2	<b>∀</b>	345.61	345.9

TZ O TZ		1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-phenyl)-urea	C15H11CIZF3N2O2	<b>4</b>	379.16	379.9
IZ O IZ TO TZ TO	<del> </del>	1-Cyclohexyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)-urea	C14H18CI2N2O2	ď	317.21	317.8
P S S S S S S S S S S S S S S S S S S S		1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethoxy-phenyl)-urea	C15H11Cl2F3N2O3	¥	395.16	395.4
IZ O IZ		1-(4-Cyano-phenyl)-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea	C15H11Cl2N3O2	A	336.18	336.4
TZ TO TZ	101	1-Benzo[1,3]dioxol-5-yl-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea	C15H12Cl2N2O4	<b>∀</b>	355.18	. 355.2

325.5	341.4	339.4	401.3	. 361.3
325.19	341.19	339.22	401.24	361.23
¥	¥	∢	A	Ą
C15H14C1ZN2O2	C15H14Cl2N2O3	C16H16Cl2N2O2	C17H18C12N2O5	C18H14Cl2N2O2
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-o-tolyl-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3-methoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2,6-dimethyl- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,4,5- trimethoxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-naphthalen-1-yl- urea
E S	D IS ON IS O		CI OMe OMe	TZ O TZ
113	114	115	116	117

369.3	403.3	311.3	349.9	320.0
369.29	403.26	311.17	349.15	319.17
<b>∢</b>	А	A	A	<b>4</b>
C18H22Cl2N2O2	C20H16C12N2O3	C14H12Cl2N2O2	C12H14BrFN2O4	C12H16BrFN2O2
1-Adamantan-1-yl-3-(3,5-dichloro- 2-hydroxy-4-methyl-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4-phenoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenyl-urea	3-[3-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-ureido]-propionic C12H14BrFN2O4 acid ethyl ester	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-pentyl-urea
	# 5 5	5 12 0 12 0		IZ TO TZ TO TZ
118	119	120	121	122

IZ O	1-Benzyl-3-(5-bromo-3-fluoro-2- hydroxy-phenyl)-urea	C14H12BrFN2O2	A	339.16	340.0
	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(2-methyl-benzyl)-urea	C15H14BrFN2O2	ď	353.19	353.9
	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-phenethyl-urea	C15H14BrFN2O2	<b>V</b>	353.19	353.9
	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	C15H22BrFN2O2	<b>∀</b>	361.25	362.0
·	1-tert-Butyl-3-(5-bromo-3-fluoro- 2-hydroxy-phenyl)-urea	C11H14BrFN2O2	<b>A</b>	305.14	305.8

r	<del></del>	· · · · · · · · · · · · · · · · · · ·	1	
346.1	407.8	394.9	359.9	393.9
345.21	407.16	394.02	359.58	393.13
¥	¥	¥	٧	¥
C14H18BrFN2O2	C15H11BrF4N2O2	C13H8BrCl2FN2O2	C13H9BrCIFN2O2	C14H9BrF4N2O2
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea
E E	THE COLUMN	HA TO THE TOTAL	HO H	F IN
128	129	130	131	132

				ь -
332.0	409.8	350.9	369.7	. 339.8
331.18	409.13	350.14	369.14	339.16
<b>∀</b>	∢	∢	¥	¥
C13H16BrFN2O2	C14H9B <del>r</del> F4N2O3	C14H9BrFN3O2	C14H10BrFN2O4	C14H12BrFN2O2
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-cyclohexyl-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(5-bromo-3-fluoro-2-hydroxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-o-tolyl-urea
	HO IN OUR STANK	75 12 5 4	TZ O TZ	12 5 12 6
133	134	135	136	137

355.5	353.6	415.6	375.6	383.7
355.16	353.19	415.21	375.19	383.26
A	∢	ď	ď	¥
C14H12BrFN2O3	C15H14BrFN2O2	C16H17BrFN2O5	C17H12BrFN2O2	C17H20BrFN2O2
1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(3-methoxy-phenyl)-	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(3,4,5-trimethoxy- phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(5-Bromo-3- fluoro-2-hydroxy-phenyl)-urea
By Children By Chi	#	Br OMe		F IN
138	139	140	141	142

12 o		1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(4-phenoxy-phenyl)-	C19H14BrFN2O3	Ą	417.23	417.6	
~-늅	1						
		1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenyl-urea	C13H10BrFN2O2	<b>∀</b>	325.13	325.7	
TZ =0	> -	3-[3-(3,5-Difluoro-2-hydroxy-phenyl)-ureido]-propionic acid ethyl ester	C12H14F2N2O4	V .	288.25	288.9	
E D	\ \{	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-pentyl-urea	C12H16F2N2O2	¥	258.26	258.9	
P IX		1-Benzyl-3-(3,5-difluoro-2- hydroxy-phenyl)-urea	C14H12F2N2O2	A	278.25	278.8	
P IN	TIZ	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	C15H14F2N2O2	V	292.28	292.9	

	<del>,</del>				
292.9	300.5	244.3	284.6	346.5	333.3
292.28	300.34	244.24	284.30	346.25	333.12
V V	¥	¥	A	Ą	¥
C15H14F2N2O2	C15H22F2N2O2	C11H14F2N2O2	C14H18F2N2O2	C15H11F5N2O2	C13H8CI2F2N2O2
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	1-tert-Butyl-3-(3,5-difluoro-2- hydroxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea
HO H	H N N N N N N N N N N N N N N N N N N N	F OH H H	F CH H H	P N N N N N N N N N N N N N N N N N N N	TIN O
149	150	151	152	153	154

298.9	332.7	270.7	348.6	289.5	308.5	278.6
298.67	332.23	270.28	348.22	289.24	308.24	278.25
A	¥	¥	. ∢	Ą	¥	Ą
C13H9CIF2N2O2	C14H9F5N2O2	C13H16F2N2O2	C14H9F2F3N2O3	C14H9F2N3O2	C14H10F2N2O4	C14H12F2N2O2
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5- difluoro-2-hydroxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-o-tolyl-urea
TZ O	IN O IN	E IN	HO THE STATE OF STATE	E S	E THE STATE OF THE	TIN TO THE TIME TO
155	156	157	158	159	160	191

 H N OMe	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	C14H12F2N2O3	¥	294.25	294.5
 P IZ	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	C15H14F2N2O2	∢	292.28	292.6
 F OMe OMe	1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	C16H17F2N2O5	∢	354.31	354.6
TN O	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea	C17H12F2N2O2	∢ .	314.29	314.6
TIN LL	1-Adamantan-1-yl-3-(3,5-difluoro- 2-hydroxy-phenyl)-urea	C17H20F2N2O2	∢	322.35	322.7
HZ O	1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(4-phenoxy-phenyl)- urea	C19H14F2N2O3	<b>V</b>	356.32	356.6

264.7	331.1	301.2	321.0	335.1
264.23	330.76	300.78	320.77	334.80
A	А	Α .	Ą	∢
C13H10F2N2O2	C14H19CIN2O5	C14H21CIN2O3	C16H17CIN2O3	C17H19CIN2O3
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-phenyl-urea	3-{3-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-ureido}-propionic acid ethyl ester	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-pentyl- urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-pentyl- urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-urea
TZ TZ TZ TZ	N HO TO	PO NO	HO HO TO	IN HO HO
168	169	170	171	172

335.3	343.7	287.6	327.5	389.4
334.80	342.86	286.75	326.82	388.77
¥	А	A	<b>V</b>	A
C17H19CIN2O3	C17HZ7Cl2N2O2	C13H19CINZO3	C16HZ3CINZO3	C17H16CIF3N2O3
1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- phenethyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-[5-chloro-2-hydroxy-3-(1-hydroxy-ethyl)- phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-urea
12 5 5 5	JZ D JZ D JZ	12 12 15 15 15	E TE	HO HO N N N N N N N N N N N N N N N N N
173	174	175	176	17.1

376.2	341.6	375.0	313.0	. 391.2
375.63	341.19	374.74	312.79	390.74
¥	А	A	V	A
C15H13Cl3N2O3	C15H14Cl2N2O3	C16H14CIF3N2O3	C15H21CIN2O3	C16H14CIF3N2O4
1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-chloro-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-cyclohexyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethoxy-phenyl)-urea
HO HO TO	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	HO HO TO	12 40 12 50 12 70 70 70 70 70 70 70 70 70 70 70 70 70	HO HO HO TO
178	179	180	181	182

332.0	351.1	321.0	337.1	. 335.2
331.75	350.75	320.77	336.77	334.80
A	Ą	Ą	A	¥
C16H14CIN3O3	C16H15CIN2O5	C16H17CIN2O3	C16H17CINZO4	C17H19CIN2O3
1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-[5-chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-o-tolyl- urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(3-methoxy-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(2,6- dimethyl-phenyl)-urea
HO HO IS	OH OH OH OF CITY OF CI	IN O HO	OH OH OHO	TN TO TO
183	184	185	186	187

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397.2	357.1	365.1	399.0	307.0
396.82	356.80	364.87	398.84	306.74
<b>∀</b>	A	•	¥	A
C18H21CIN2O6	C19H17CIN2O3	C19H25CIN2O3	C21H19CIN2O4	C15H15GIN2O3
1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(3,4,5-trimethoxy-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-[5-chloro-2- hydroxy-3-(1-hydroxy-ethyl)- phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-phenoxy-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-phenyl- urea
H HO	\$ 5 0 TZ	P	FO TO	HO HO TO
188	189	190	191	192

-Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -Ω -	1-(5-Chloro-2-hydroxy-phenyl)-3- pentyl-thiourea	C12H17CINZOS	I	272.79	272.9
TZ S	1-Benzyl-3-(5-chloro-2-hydroxy- phenyl)-thiourea	C14H13CINZOS	Ι	292.78	293.1
TZ S	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	C15H15GIN2OS	I	306.81	306.9
H S S	1-(5-Chloro-2-hydroxy-phenyl)-3- phenethyl-thiourea	C15H15CIN2OS	I	306.81	307.1
P N N N N N N N N N N N N N N N N N N N	1-(5-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23CIN2OS	I	314.87	315.0

		· · · · · · · · · · · · · · · · · · ·		
258.9	245.0	299.1	361.1	347.9
258.77	244.74	298.83	360.78	347.65
I	I	·	Н	н
C11H15CIN2OS	C10H13CIN2OS	C14H19GIN2OS	C15H12CIF3N2OS	C13H9Cl3N2OS
1-tert-Butyl-3-(5-chloro-2- hydroxy-phenyl)-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea
IZ SIZ SIZ	₽—	5——5	PE STEE STEE STEE STEE STEE STEE STEE ST	5 12 8 12 8
198	199	200	201	202

203	5 12 5 5	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	C13H10Cl2N2OS	pent	313.20	313.5	
	45°	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10CIF3N2OS	П	346.76	347.0	
l	g − Ω IZ IZ O	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea	C13H17CINZOS	I	284.80	285.0	
1	12 12 12 12 12 12	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	C14H10CIF3N2OS	I	346.76	347.0	
I	TZ S	1-(5-Chloro-2-hydroxy-phenyl)-3- phenyl-thiourea	C13H11CINZOS	1	278.76	. 279.0	

307.5	327.4	341.4	341.5	349.6
307.24	327.23	341.26	341.26	349.32
П	I	1	H	I
C12H16CIZN2OS	C14H12Cl2N2OS	C15H14Cl2N2OS	C15H14Cl2N2OS	C15H22Cl2N2OS
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(2-methyl-benzyl)-thiourea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea
		P D D	TIN TO TO	TZ S
208	500	210	211	212

213	H S S S S S S S S S S S S S S S S S S S	1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-phenyl)-thiourea	C11H14Cl2N2OS	H	293.21	293.6
214	Col No	1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	C10H12CI2N2OS	m	279.19	279.5
215	PO TO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	C14H18Cl2N2OS	P=4	333.28	333.5
216	CI OH H N N CIF3	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	CISHIICIZF3N2OS	ы	395.23	395.5
217	CO H H CO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- thiourea	C13H8Cl4N2OS	<b>P-4</b>	382.09	382.3

218	2 ZZ	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	C13H9CI3N2OS	I	345.65	345.9
219	P D D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	C14H9Cl2F3N2OS	I	381.2	381.6
220	TIN TO TO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16Cl2N2OS	I	319.25	319.6
221	E SIN	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9Cl2F3N2OS	I	381.20	381.4
222	TN TO TO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenyl-thiourea	C13H10Cl2N2OS	I	313.20	. 313.5
223	D IN IN S	1-(3-Chloro-2-hydroxy-phenyl)-3- pentyl-thiourea	C12H17CIN2OS	I	272.79	273.2

224	CI OH NH S	1-Benzyl-3-(3-chloro-2-hydroxy- phenyl)-thiourea	C14H13CIN2OS	Ι	292.78	293.1
225	CI H H HO IO	1-(3-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	C15H15CIN2OS	I	306.81	307.0
226	N H HO TO	1-(3-Chloro-2-hydroxy-phenyl)-3- phenethyl-thiourea	C15H15CIN2OS	Ι	306.81	307.1
227	HO HO ID	1-(3-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23CIN2OS	Ι	314.87	315.2
228	CI N N N N N N N N N N N N N N N N N N N	1-tert-Butyl-3-(3-Chloro-2- hydroxy-phenyl)-thiourea	C11H15CIN2OS	I	258.77	259.0
229	CI CI H	1-(3-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	C10H13CIN2OS	I	244.74	244.9
230	S H HO	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	C14H19CIN2OS	I	298.83	299.3

361.1	348.0	313.5	347.2	285.1	347.2	279.0
360.78	347.65	313.20	346.76	284.8	346.76	278.76
н	I	I	I	I	I	I
CISH12CIF3N2OS	C13H9Cl3N2OS	C13H10Cl2N2OS	C14H10CIF3N2OS	C13H17CINZOS	C14H10ClF3N2OS	CI3H11CINZOS
1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- phenyl-thiourea
OH H N N N N N N N N N N N N N N N N N N	CI OH II OH	HN S HO S S S S S S S S S S S S S S S S S	CI N H N CF3	D HO HO S	D S N S N S N S N S N S N S N S N S N S	TZ S TZ S
231	232	233	234	235	236	237

238	HN HN S	1-(3-Fluoro-2-hydroxy-phenyl)-3- pentyl-thiourea	C12H17FN2OS	I	256.34	256.8
239	HO HO S	1-Benzyl-3-(3-fluoro-2-hydroxy- phenyl)-thiourea	C14H13FN2OS	I	276.33	276.7
240	H H N S	1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	C15H15FN2OS	I	290.36	290.5
241	N N N N N N N N N N N N N N N N N N N	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenethyl-thiourea	C15H15FN2OS	I	290.36	290.5
242	P H H N H N N N N N N N N N N N N N N N	1-(3-Fluoro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23FN2OS	· I	298.42	298.7
243	HO HO S	1-tert-Butyl-3-(3-fluoro-2- hydroxy-phenyl)-thiourea	C11H15FN2OS	Н	242.31	242.8
244	F N S	1-(3-Fluoro-2-hydroxy-phenyl)-3- isopropyl-thiourea	C10H13FN2OS	П	228.29	228.5

282.7	344.7	331.5	297.1	330.6	268.6
282.38	344.33	331.19	296.75	330.30	268.35
	H		<b>-</b>	-	Н
C14H19FN2OS	C15H12F4N2OS	C13H9CIZFN2OS	C13H10CIFN2OS	C14H10F4N2OS	CI3H17FN2OS
1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea
HO HO S	F H H CF3	NH N	HA STAN	F OH H N S OF S	FINAL SERVICE
245	246	247	248	249	250

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330.5	262.5	321.8	341.5	355.6	355.6
330.30	262.30	321.27	341.26	355.28	355.28
I	I	П	H	-	I
C14H10F4N2OS	C13H11FN2OS	C13H18CI2N2OS	C15H14CI2N2OS	C16H16Cl2N2OS	C16H16Cl2N2OS
1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)- thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2-methyl- benzyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenethyl- thiourea
F OH N OF 3	F OH N N	CI OH N N N	Q OH NH CH	D HN S HN S	TX TO TO TO THE TABLE TO THE TA
251	252	253	254	255	256

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363.6	307.5	293.6	347.5	409.5
363.35	307.24	293.21	347.30	409.25
Н	П			П
C16H24CIZN2OS	C12H16CI2N2OS	C11H14Cl2N2OS	C15H20C12N2OS	C16H13Cl2F3N2OS
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(1,1,3,3- teframethyl-butyl)-thiourea	1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)- thiourca	1-(5-Chloro-2-hydroxy-4-methyl- phenyl)-3-isopropyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3- cyclohexylmethyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-benzyl)-thiourea
N N N N N N N N N N N N N N N N N N N	HN S IN IS	CO N N N N N N N N N N N N N N N N N N N	OH NH S NH S	CI OH N N N N N N N N N N N N N N N N N N
257	258	259	260	261

396.3	361.9	395.7	333.8	. 395.8
396.12	361.67	395.23	333.28	395.23
-	П		н	-
C14H10C14N2OS	C14H11Cl3N2OS	C15H11Cl2F3N2OS	C14H18CI2N2OS	C15H11Cl2F3N2OS
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,5-dichloro- phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4-chloro- phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-cyclohexyl- thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2- trifluoromethyl-phenyl)-thiourea
		C C C C C C C C C C C C C C C C C C C	D TN S TN S	PN PS
262	263	264	265	566

327.23	335.24 335.8	355.23 355.4	369.25 369.5	369.25 369.5
I 32	I 33	I 35	I 36	)9E I
C14H12CI2N2OS	C12H16BrFN2OS	C14H12BrFN2OS	C15H14BrFN2OS	C15H14BrFN2OS
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenyl-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(5-bromo-3-fluoro-2- hydroxy-phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenethyl-thiourea
H N N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N	HO HO NEW YORK NEW YO	PA P	FO STANCE OF THE
267	268	269	270	271

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	377.5	321.5	307.4	361.5	423.5
	377.32	321.21	307.19	361.28	423.23
	I	н	<b>-</b>		I
	C15H22BrFN2OS	C11H14BrFN2OS	C10H12BrFN2OS	C14H18BrFN2OS	C15H11BrF4N2OS
	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-thiourea	1-tert-Butyl-3-(5-bromo-3-fluoro- 2-hydroxy-phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-isopropyl-thiourea	1-(5-Bromo-3-fiuoro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(4-trifluoromethyl-benzyl)-thiourea
	IN N	HO S IN S	IN I	HN N N N N N N N N N N N N N N N N N N	P. N. S. M. S.
	272	273	274	275	276

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410.5	375.9	409.5	347.6	. 409.5
410.09	375.65	409.20	347.25	409.20
H	I	1		Н
C13H8BrCl2FN2OS	C13H9BrCIFN2OS	C14H9BrF4N2OS	C13H16B#N2OS	C14H9BrF4N2OS
1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-cyclohexyl-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea
HO H	HA NA	Property of the state of the st	N N N N N N N N N N N N N N N N N N N	HN FIN S
277	278	279	280	281

341.5	274.8	294.7	308.6	308.6	316.8
341.20	274.33	294.32	308.35	308.35	316.41
I	I	Ι	I	Ι	I
C13H10BrFN2OS	C12H16F2N2OS	C14H12F2N2OS	C15H14F2N2OS	C15H14F2N2OS	C15H22F2N2OS
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenyl-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,4-difluoro-2- hydroxy-phenyl)-thiourea	1-(3,4-Diffuoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,4-Difluoro-2-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea
N N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N	P H H H	F H H N N N N N N N N N N N N N N N N N	F OH H N	H H H H H H H H H H H H H H H H H H H
282	283	284	285	286	287

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260.5	246.5	300.6	362.8	349.7	315.2
260.30	246.28	300.37	362.32	349.18	314.74
ı	I	I	<b>p</b> -c-d	Н	I
C11H14P2N2OS	C10H12F2N2OS	C14H18F2N2OS	C15H11F5N2OS	C13H8Cl2F2N2OS	C13H9CIF2N2OS
1-tert-Butyl-3-(3,4-Difluoro-2- hydroxy-phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-isopropyl-thiourea	1-(3,4-Diffuoro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- thiourea	1-(3,4-Difluoro-2-hydroxy-phenyl)-3-(4-chloro-phenyl)-thiourea
JIZ S	HO H	HZ HZ S	F CP3	THE STATE OF THE S	FIN SO
288	289	290	291	292	293

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348.8	286.6	348.8	280.5	316.9	337.2
348.29	286.34	348.29	280.29	316.85	336.84
I	П	Н	ı	H	I
C14H9F5N2OS	C13H16F2N2OS	C14H9F5N2OS	C13H10F2N2OS	C14H21CIN2O2S	C16H17CIN2O2S
1-(3,4-Diffuoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-cyclohexyl-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-phenyl-thiourea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-pentyl-thiourea	1-Benzyl-3-[5-chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-thiourea
F OH N CF3	TN S TN	OH N S N S N S N S N S N S N S N S N S N	P N N N N N N N N N N N N N N N N N N N	PHO HO TO	5 - 5 - 5 - 5
294	295	296	297	298	299

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
300	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-thiourea	C17H19CINZO2S	I	350.86	351.1
301	FZ SS	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- phenethyl-thiourea	C17H19CIN2O2S	I	350.86	351.0
302	TZ SO TO	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-teframethyl-butyl)-thiourea	C17HZ7CINZO2S	. I	358.93	359.2
303	TZ SS TS	1-tert-Butyl-3-[5-chloro-2- hydroxy-3-(1-hydroxy-ethyl)- phenyl]-thiourea	C13H19CINZO2S	I	302.82	303.0
304	HO TIZES	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- isopropyl-thiourea	C12H17CINZO2S	I	288.79	289.0

OH OH N H 1-[5-Chi hydroxy- cyclohex	1-[5-Chle hydroxy- cyclohex	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- cyclohexylmethyl-thiourea	C16H23CIN2O2S	П	342.88	343.1
OH OH N N N S		1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- trifluoromethyl-benzyl)-thiourea	C17H16CIF3N2O2S	П	. 404.83	405.2
OH O	- 4	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(3,5- dichloro-phenyl)-thiourea	CISH13CI3N2O2S	щ	391.70	392.0
N HO HO IO	1 4 0	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-thiourea	C15H14Cl2N2O2S	н	357.25	357.6
OH OH N H 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	<u> </u>	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	Ι	390.81	391.0

<b>—</b>	H H H	1 6 Chloss 2 hudmon; 2 (1-				
	∑ ≥ ∞ ≥ ~ 5	hydroxy-ethyl)-phenyl]-3- cyclohexyl-thiourea	C15H21CIN2O2S	I	328.86	329.4
i	₽ - 2	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(2-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	I	390.81	391.0
	P S S S S S S S S S S S S S S S S S S S	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-phenyl- thiourea	C15H15CINZOZS	I	322.81	323.1
l	FZ 5	4-Chloro-2-(2-phenylsulfanyl- benzylamino)-phenol	C19H1¢CINOS	D	341.85	342.2
	TZ 5	4-Chloro-2-(2-p-tolylsulfanyl-benzylamino)-phenol	C20H18CINOS	D	355.88	356.3

376.8	387.2	372.4	376.8	376.8
, in	ñ			
376.30	386.85	371.88	376.30	376.30
D	Q	Q	Q	Q
C19H15Cl2NOS	C19H15CINZO3S	C20H18CINO2S	C19H15CIZNOS	C19H15Cl2NOS
4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	4-Chloro-2-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	4-Chloro-2-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	4-Chloro-2-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	4-Chloro-2-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol
5 -5 -5	12 5 0 0 0	The second secon	₹	5 5 5 5
315	316	317	318	319

411.2	399.3	393.4	421.7
410.74	398.91	392.90	421.30
Q	Q	Q	Q
C19H14Cl3NOS	C21H19CIN2O2S	C22H17CIN2OS	C19H14CIZNZO3S
4-Chloro-2-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(5-Chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	4-Chloro-2-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-Chloro-2-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol
2 -2 -2	OH NHAC		S T T T T T T T T T T T T T T T T T T T
320	321	322	323

401.2	391.9	408.7	376.7
400.88	391.31	408.30	376.30
A	Q	<b>Q</b>	Ω
C20H17CIN2O3S	C19H16Cl2N2OS	C19H15CI2NO3S	C19H15Cl2NOS
4-Chloro-2-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- chloro-phenol	4-Chloro-2-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	2,4-Dichloro-6-(2-phenylsulfanyl- benzylamino)-phenol
δ	IN HO IS	The state of the s	TZ TO TO
324	325	326	327

390.7	411.1	421.8	406.7	411.2
390.33	410.75	421.30	406.33	410.75
Ω	D	D	D	Q
C20H17Ci2NOS	C19H14Cl3NOS	C19H14Cl2N2O3S	C20H17Cl2NO2S	C19H14Cl3NOS
2,4-Dichloro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	2,4-Dichloro-6-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2,4-Dichloro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(2-chloro- phenylsulfanyl)-benzylamino]- phenol
12 5 5	72 5 5 5	EN TO	E S	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
328	329	330	331	332

411.2	445.6	433.8	427.8
410.75	445.19	433.36	427.35
D	D	Q	Q
C19H14Cl3NOS	C19H13Cl4NOS	C21H18Cl2N2O2S	C22H16Cl2N2OS
2,4-Dichloro-6-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
5 5 5 5	D D D D D	G OH NHAC	S TN TO
333	334	335	336

456.0	435.7	426.0	443.1
455.74	435.33	425.76	442.75
Q	Ω.	Q	Q
C19H13Cl3N2O3S	C20H16Cl2N2O3S	C19H15Cl3N2OS	C19H14Cl3NO3S
2,4-Dichloro-6-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,4-Dichloro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4,6- dichloro-phenol	2,4-Dichloro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
A P P P P P P P P P P P P P P P P P P P	SON HO TO	C C C C C C C C C C C C C C C C C C C	SSC O
337	338	339	340

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342.3	356.3	376.7	387.2	372.2
341.85	355.88	376.30	386.85	371.88
А	Q	Q	Q	Ω
C19H16CINOS	C20H18CINOS	C19H15CIZNOS	C19H15CIN2O3S	C20H18CINO2S
2-Chloro-6-(2-phenylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Chloro-6-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Chloro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Chioro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TIN TO	TN TO	O P N N N N N N N N N N N N N N N N N N	CI OH NO2	S HA POWO
341	342	343	344	345

376.8	376.8	411.0	399.3	393.4
376.30	376.30	410.74	398.91	392.90
Q	Q	Q	Q	Ð
C19H15ClZNOS	C19H15CIZNOS	C19H14Cl3NOS	C21H19CIN2O2S	C22H17CIN2OS
2-Chloro-6-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-6-[2-(3-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Chloro-6-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2-Chloro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
COLUMN SECTION OF THE PROPERTY	CI OH N	D S S D	CI OH K	THE SECOND SECON
346	347	348	349	350

421.5	401.3	392.4	408.6
421.30	400.88	391.31	408.30
Q	Q .	Q	A
C19H14Cl2N2O3S	C20H17CIN2O3S	C19H16Cl2N2OS	C19H15Cl2NO3S
2-Chloro-6-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-phenol	2-Chloro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- chloro-phenol	2-Chloro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
12 5 12 5	ON TIN	Z-T-Z-V-S-T-Z-V-S-T-Z-V-S-V-S-V-S-V-S-V-S-V-S-V-S-V-S-V-S-V	TIN TO
351	352	353	354

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324.6	340.8	360.1	370.8	355.8
325.40	339.43	359.84	370.40	355.43
Q	Q	О	Q	О
C19H16FNOS	C20H18FNOS	C19H15CIFNOS	C19H15FN2O3S	C20H18FNO2S
2-Fluoro-6-(2-phenylsulfanyl- benzylamino)-phenol	2-Fluoro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Fluoro-6-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
F - S	N HO S	TN TO	E S S NO2	P OMe
355	356	357	358	359

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360.2	360.3	394.6	382.9	377.0
359.84	359.84	394.29	382.45	376.45
A	Q	Q	Q	A
C19H15CIFNOS	C19H15CIFNOS	C19H14Cl2FNOS	C21H19FN2O2S	C22H17FN2OS
2-Fluoro-6-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-6-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-6-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Fluoro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2-Fluoro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
HZ S	HA S	HA S	F OH H	TZ SS
360	361	362	363	364

405.3	384.9	375.1	392.0
404.84	384.42	374.86	391.84
Q	A	<b>.</b>	Q
C19H14CIFN2O3S	C20H17FN2O3S	C19H16CIFN2OS	C19H15CIFNO3S
2-Fluoro-6-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-phenol	2-Fluoro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- fluoro-phenol	2-Fluoro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
P S S S S S S S S S S S S S S S S S S S	PON TEN S	THE SECOND SECON	E SZO
365	366	367	398

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390.6	404.6	425.2	435.8	420.6
390.33	404.35	424.77	435.32	420.35
Д	Q	Q	Q	Q
C20H17CIZNOS	C21H19CIZNOS	C20H16Cl3NOS	C20H16Cl2N2O3S	C21H19Cl2NO2S
2,4-Dichloro-3-methyl-6-(2-phenylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-[2-(4- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TX 5	HN HO IS	IN TO	CI OH NO2	P P P P P P P P P P P P P P P P P P P
369	370	371	372	373

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425.1	425.1	459.5	447.8	441.6
424.77	424.77	459.22	447.38	441.37
Q	А	Д	Ω	Q
C20H16Cl3NOS	C20H16Ci3NOS	C20H15C!4NOS	C22H20Cl2N2O2S	C23H18Cl2N2OS
2,4-Dichloro-3-methyl-6-[2-(2- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(3- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-2-hydroxy-4-methyl-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-3-methyl-6-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenol
TN TO	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	CI CI S	
374	375	376	377	378

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470.0	449.6	439.9	457.0
469.77	449.35	439.79	456.77
Q	Q	Q	D
C20H15Cl3N2O3S	C21H18Cl2N2O3S	C20H17Cl3N2OS	C20H16Cl3NO3S
2,4-Dichloro-3-methyl-6-[2-(4- chloro-phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-(5-nitro- 2-p-tolylsulfanyl-benzylamino)- phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4,6- dichloro-5-methyl-phenol	2,4-Dichloro-3-methyl-6-[2-(4- chloro-benzenesulfonyl)- benzylamino]-phenol
D TZ		P P P P	S S S S S S S S S S S S S S S S S S S
379	380	381	382

					-	
IZ		4-Bromo-2-fluoro-6-(2-phenylsulfanyl-benzylamino)-phenol	C19H15BrFNOS	Q	404.30	404.7
===		4-Bromo-2-fluoro-6-(2-p-tolylsulfanyl-benzylamino)-phenol	C20H17BrFNOS	Д	418.33	418.6
	5	4-Bromo-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-fluoro-phenol	C19H14BrCIFNOS	D	438.74	439.0
IZ	S S S S S S S S S S S S S S S S S S S	4-Bromo-2-fluoro-6-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	C19H14BrFN2O3S	Ω	449.30	449.8
IZ	B B B B B B B B B B B B B B B B B B B	4-Bromo-2-fluoro-6-[2-(4- methoxy-phenylsulfanyl)- benzylamino]-phenol	C20H17BrFNO2S	О	434.33	434.7

439.2	439.1	473.6	461.8	455.7
438.74	438.74	473.19	461.35	455.35
Q	D	О	Ω	Q
C19H14BrCIFNOS	C19H14BrCIFNOS	C19H13BrCIZFNOS	C21H18BrFN2O2S	C22H16BrFN2OS
4-Bromo-2-[2-(2-chloro- phenylsulfanyl)-benzylamino]-6- fluoro-phenol	4-Bromo-2-[2-(3-chloro-phenylsulfanyl)-benzylamino]-6-fluoro-phenol	4-Bromo-2-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]-6- fluoro-phenol	N-(4-{2-[(5-Bromo-3-filuoro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	4-Bromo-2-fluoro-6-[2-(quinolin- 7-ylsulfanyl)-benzylamino]-phenol
5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	5 S S S S S S S S S S S S S S S S S S S	E S S	Br S	
388	389	390	391	392

484.1	463.7	454.1	471.2
483.74	463.32	453.76	470.74
Q	D	Q	Q
C19H13BrCIFN2O3 S	C20H16BrFN2O3S	C19H15BrCIFN2OS	C19H14BrCIFNO3S
4-Bromo-2-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-6-fluoro-phenol	4-Bromo-2-fluoro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- bromo-6-fluoro-phenol	4-Bromo-2-[2-(4-chloro-benzenesulfonyl)-benzylamino]-6-fluoro-phenol
SON		1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	TZ TO TO
393	394	395	396

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343.6	357.8	378.1	388.8	373.7
343.39	357.42	377.83	388.39	373.42
D	D	Q	Ω	D
C19H15F2NOS	C20H17F2NOS	C19H14CIF2NOS	C19H14F2N2O3S	C20H17F2NO2S
2,3-Difluoro-6-(2-phenylsulfanylbenzylamino)-phenol	2,3-Difluoro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	6-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2,3-difluoro-phenol	2,3-Difluoro-6-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	2,3-Difluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
12 15 10 112 112 112	TZ TO TE	TZ TO TE TO	TZ TO L	TZ S S S S S S S S S S S S S S S S S S S
397	398	399	400	401

402	### DE TEXT   10   10   10   10   10   10   10   1	6-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2,3-difluoro-phenol	C19H14CIF2NOS	Q	377.83	378.1
403	FO. SO. SO. SO. SO. SO. SO. SO. SO. SO. S	6-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2,3-difluoro-phenol	C19H14CIF2NOS	Q	377.83	378.2
404	4	6-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2,3- difluoro-phenol	C19H13Cl2F2NOS	O	412.28	412.6
405	NITAC SHITAC	N-(4-{2-[(3,4-Difluoro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	C21H18F2N2O2S	Д	400.44	400.8
406	TZ TO LL	2,3-Difluoro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	C22H16F2N2OS	D	394.44	394.9

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423.3	402.8	393.0	392.3
422.83	402.41	392.85	391.84
D	Q	D	Q
C19H13CIF2NZO3S	C20H16F2N2O3S	C19H15CIF2N2OS	C19H14CIF2NO3S
6-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2,3-difluoro- phenol	2,3-Difluoro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	6-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2,3- difluoro-phenol	6-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-2,3-difluoro-phenol
DE STEEL STE	P P P P P P P P P P P P P P P P P P P	TX TX TX	TN Sto
407	408	409	410

386.4	400.2	420.9	431.3	416.3
385.91	399.93	420.35	430.90	415.93
D	D	Q	A	Q
C21H20CINO2S	C22H22CINO2S	C21H19Cl2NO2S	C21H19CIN2O4S	C22H22CINO3S
4-Chloro-2-(1-hydroxy-ethyl)-6- (2-phenylsulfanyl-benzylamino)- phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- (2-p-tolylsulfanyl-benzylamino)- phenol	4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(4-nitro-phenylsulfanyl)- benzylamino]-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(4-methoxy-phenylsulfanyl)- benzylamino]-phenol
12 5 5	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	5 5 5 5 5	TZ HO ON TZ HO ON	4 4 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
411	412	413	414	415

P - 2	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	4-Chloro-2-[2-(2-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H19Cl2NO2S	Д	420.35	420.9	
5—5 5—5	5	4-Chloro-2-[2-(3-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H19CIZNO2S	Д	420.35	420.8	
₽ - 2	5 5	4-Chloro-2-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-efhyl)-phenol	C21H18Cl3NO2S	Д	454.80	455.2	
₹————————————————————————————————————	S NHA	N-[4-(2-{[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenylamino]-methyl}-phenylsulfanyl)-phenyl]-acetamide	C23H23CIN2O3S	О	442.96	443.4	
₹——¤	z	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(quinolin-7-ylsulfanyl)- benzylamino]-phenol	C24H21CIN2O2S	Q	436.95	437.3	

465.9	445.3	435.6	452.5
465.35	444.93	435.37	452.35
D	Q	Q	Q
C21H18Cl2N2O4S	C22H21CIN2O4S	C21H20Cl2N2O2S	C21H19CI2NO4S
4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- (5-nitro-2-p-tolylsulfanyl- benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- chloro-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-[2-(4-chloro- benzenesulfonyl)-benzylamino]-6- (1-hydroxy-ethyl)-phenol
D HO HO HO HO HO HO HO HO HO HO	DE TEX	1 N N N N N N N N N N N N N N N N N N N	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
421	422	423	424

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337.8	351.8	371.9	382.7	367.9
337.44	351.46	371.88	382.43	367.46
D	Q	D	Q	Q
C20H19NO2S	C21H21NO2S	C20H18CINO2S	C20H18N2O4S	C21H21N03S
2-Hydroxymethyl-6-(2- phenylsulfanyl-benzylamino)- phenol	2-Hydroxymethyl-6-(2-p-tolyisulfanyl-benzylamino)-phenol	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-6-hydroxymethyl- phenol	2-Hydroxymethyl-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Hydroxymethyl-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
# # # # # # # # # # # # # # # # # # #	TZ TZ	12 5 5	F. S.	HO HO HO
425	426	427	428	429

430	# 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-6-hydroxymethyl- phenol	C20H18CINO2S	Q	371.88	371.9
431	E S	2-[2-(3-Chloro-phenyisulfanyl)- benzylamino]-6-hydroxymethyl- phenol	C20H18CINO2S	D	371.88	371.9
432	5 5 5 5	2-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-6- hydroxymethyl-phenol	C20H17Cl2NO2S	. О	406.33	406.5
433	NHAe	N-(4-{2-[(2-Hydroxy-3- hydroxymethyl-phenylamino)- methyl]-phenylsulfanyl}-phenyl)- acetamide	C22H22N2O3S	Ω	394.49	349.9
434	TZ 5	2-Hydroxymethyl-6-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	C23H20N2O2S	Q	388.48	388.8

417.2	396.8	387.1	44.0
416.88	396.46	386.90	403.88
Q	Q	Ω	α
C20H17CIN2O4S	C21H20N2O4S	C20H19CIN2O2S	C20H18CINO4S
2-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-6- hydroxymethyl-phenol	2-Hydroxymethyl-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-6-hydroxymethyl-phenol	2-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-6-hydroxymethyl- phenol
S HO HO	S HO HO	THE HOLD .	S ₂ O HO HO
435	436	437	438

390.5	418.7	439.0	449.7	434.6
390.33	418.37	438.79	449.34	434.37
D	D	O.	Ω	A
C21H19Cl2NOS	C22H21Cl2NOS	C21H18CJ3NOS	C21H18CI2N2O3S	C22H21Cl2NO2S
2,4-Dichloro-3-ethyl-6-(2- phenylsulfanyl-benzylamino)- phenol	2,4-Dichloro-3-ethyl-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-cthyl-6-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2,4-Dichloro-3-ethyl-6-[2-(4- methoxy-phenylsulfanyl)- benzylamino]-phenol
	5 5 5	2 Z	PO DO	TO T
439	440	441	442	443

438.9	438.9	473.5	461.6	455.7
438.79	438.79	473.24	461.40	455.39
О	Ω	Ω	Ω	Q
C21H18CI3NOS	C21H18Cl3NOS	C21H17CI4NOS	C23H22Cl2N2O2S	C24H20Cl2N2OS
2,4-Dichloro-3-ethyl-6-[2-(2- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-cthyl-6-[2-(3- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-[2-(3,4- dichloro-phenylsulfanyl)- benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-4-ethyl-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-3-ethyl-6-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenol
5 5 5	2 ZZ		CI C	
444	445	446	447	448

	15		
484.0	463.5	454.1	471.0
483.79	463.37	453.81	470.79
Q	Ω	Q	Q
C21H17Cl3N2O3S	C22H20CI2N2O3S	C21H19CI3N2OS	C21H18CI3NO3S
2,4-Dichloro-3-ethyl-6-[2-(4- chloro-phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-4,6-dichloro-5-ethyl-phenol	2,4-Dichloro-3-ethyl-6-[2-(4- chloro-benzenesulfonyl)- benzylamino]-phenol
\$\frac{1}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac{5}{5}\frac	20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
449	450	451	452

<del> </del>	HOOC OH	2-Hydroxy-3-(2-phenylsulfanyl- benzylamino)-benzoic acid	C20H17NO3S	D	351.42	351.6
	HOOCH HOOCH	2-Hydroxy-3-(2-p-tolylsulfanyl- benzylamino)-benzoic acid	C21H19NO3S	D	365.44	365.8
	HOOOO NAME OF THE PART OF THE	3-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	C20H16CINO3S	Q	385.86	385.1
	HOOC NA	2-Hydroxy-3-[2-(4-nitro- phenylsulfanyl)-benzylamino]- benzoic acid	C20H16N2O5S	Q	396.11	396.4
	HOOC SHOWS	2-Hydroxy-3-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-benzoic acid	C21H19NO4S	Q	381.44	381.6

386.0	386.0	420.7	408.7	402.8
385.86	385.86	420.31	408.47	402.46
Q	Q	О	Q	Q
C20H16CINO3S	C20H16CINO3S	C20H15Cl2NO3S	C22H20N2O4S	C23H18N2O3S
3-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	3-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	3-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- hydroxy-benzoic acid	3-[2-(4-Acetylamino-phenylsulfanyl)-benzylamino]-2-hydroxy-benzoic acid	2-Hydroxy-3-[2-(quinolin-7- ylsulfanyl)-benzylamino]-benzoic acid
HOOOC	HOOC	HOOC NH	HOOC NHAC	HOOC PART OF THE P
458	459	460	461	462

430.9	410.7	387.2	404.1
430.86	410.44	386.90	403.88
Д	Q	Q	Q
C20H15CIN2OSS	C21H18N2OSS	C20H19CIN2O2S	C20H16CINOSS
3-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-hydroxy- benzoic acid	2-Hydroxy-3-(5-nitro-2-p-tolylsulfanyl-benzylamino)-benzoic acid	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-6-hydroxymethyl-phenol	3-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-benzoic acid
HOOC NO	HOOO TIN TIN TIN TIN TIN TIN TIN TIN TIN TIN	THE TOOCH	HOOOC HOOOC
463	464	465	466

370.8	384.9	405.0	415.8	400.9
370.40	384.43	404.84	415.40	400.43
D	D	D	Q	Q
C19H15FN2O3S	C20H17FN2O3S	C19H14CIFN2O3S	C19H14FN3O5S	C20H17FN2O4S
2-Fluoro-4-nitro-6-(2- phenylsulfanyl-benzylamino)- phenol	2-Fluoro-4-nitro-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-6-fluoro-4-nitro- phenol	2-Fluoro-4-nitro-6-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-4-nitro-phenol
TZ ON	TZ S	TZ GY	NO2 NO2	NO ₂ S
467	468	469	470	471

405.0	405.0	439.9	427.9	421.6
404.84	404.84	439.29	427.45	421.45
Q	Д	Q	D	О
C19H14CIFN2O3S	C19H14CIFN2O3S	C19H13Cl2FNZO3S	C21H18FN3O4S	C22H16FN3O3S
2-[2-(2-Chloro-phenylsulfanyl)-benzylamino]-6-fluoro-4-nitro-phenol	2-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-6-fluoro-4-nitro- phenol	2-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-6- fluoro-4-nitro-phenol	N-(4-{2-[(3-Fluoro-2-hydroxy-5- nitro-phenylamino)-methyl]- phenylsulfanyl}-phenyl)-acetamide	2-Fluoro-4-nitro-6-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol
TZ S	HZ SAL	TZ ON	NO ₂ S NHAC	TZ S
472	473	474	475	476

477	Part of the second seco	2-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-6-fluoro-4- nitro-phenol	C19H13CIFN3O5S	Д	449.84	450.1
478	TZ SON	2-Fluoro-4-nitro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	C20H16FN3O4S	Q	429.42	429.8
479	HO CON	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- fluoro-4-nitro-phenol	C19H15CIFN3O2S	Д	419.86	420.2
480	TX SO	2-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-6-fluoro-4-nitro- phenol	C19H15CIFN2O5S	Д	436.84	437.1

481	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2,4-Dichloro-6-(3-phenoxy- benzylamino)-phenol	C19H15Cl2NO2	D	360.23	360.5
482	5 5 5	2,4-Dichloro-6-[3-(4-chloro- phenoxy)-benzylamino]-phenol	C19H15Cl3NO2	Q	394.68	. 395.0
483	TZ TO TO TO TO TO TO TO TO TO TO	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-4,6-dichloro-phenol	C23H23Cl2NO2	Q	416.34	416.8
484	12X 5-05	2-(3-Benzyloxy-benzylamino)-4,6- dichloro-phenol	C20H17Cl2NO2	Q	374.26	374.6

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ပ်	\$	2-(2-Benzyloxy-benzylamino)-4,6- dichloro-phenol	C20H17Cl2NO2	Q	374.26	374.6
ပ်	5—~~~	2,4-Dichloro-6-[(naphthalen-1- ylmethyl)-amino]-phenol	C17H13Cl2NO	D	318.20	318.6
ဗ်	FZ TZ	2,4-Dichloro-6-(4-methylsulfanyl-benzylamino)-phenol	C14H13Cl2NOS	Q	314.23	314.7
	TZZ 5	2,4-Dichloro-6-(2-ethylsulfanylbenzylamino)-phenol	C15H15Cl2NOS	Q	328.26	328.6
	±z ₹	2,4-Dichloro-6-(2-morpholin-4-yl-benzylamino)-phenol	C17H18Cl2N2O2	Ω	353.24	353.6

490	E S S	2,4-Dichloro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	C17H12Cl3NOS2	D	416.77	416.9
491	Z Z Z Z Z	2,4-Dichloro-6-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	C16H13Cl2N3O	Q	334.20	334.6
492	CI OH S	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro- phenol	C11H8BrCl2NOS	О	353.06	353.4
493	5 -5 -5	2,4-Dichloro-6-[3-(4-methoxy-phenoxy)-benzylamino]-phenol	C20H17Cl2NO3	Q	390.26	390.6
494	12 5 5	2,4-Dichloro-6-(3-methyl- benzylamino)-phenol	C14H13Cl2NO	D	282.17	282.4

	FIN TO	2.4-Dichloro-6-(3-trifluoromethyl-		6	7	3 766
495		benzylamino)-phenol	C14H10ClZF3NO	a	530.14	
496	5 5 5 5	2,4-Dichloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	C13H9Cl3FNO	Q	320.57	320.8
497	5—5	2,4-Dichloro-3-methyl-6-(3- phenoxy-benzylamino)-phenol	C20H17Cl2NO2	D	374.26	374.6
498	5—5 5—5	2,4-Dichloro-3-methyl-6-[3-(4- chloro-phenoxy)-benzylamino]- phenol	C20H17Cl3NO2	Q	408.71	409.2

430.5	388.6	388.6	332.6
430.37	388.29	388.29	332.23
D	Q	Q	Q
C24H25Cl2NO2	C21H19Cl2NO2	C21H19ClZNO2	C18H15Cl2NO
2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-4,6-dichloro-3- methyl-phenol	2-(3-Benzyloxy-benzylamino)-4,6- dichloro-3-methyl-phenol	2-(2-Benzyloxy-benzylamino)-4,6- dichloro-3-methyl-phenol	2,4-Dichloro-3-methyl-6- [(naphthalen-1-ylmethyl)-amino]- phenol
2 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	5 - 5 - 5	TZ TZ TZ	5 0 5
499	200	501	502

328.6	342.8	367.6	431.2	348.8
328.26	342.29	367.27	430.80	348.23
D	Q	Q	Ω	Q
C15H15Cl2NOS	C16H17Cl2NOS	C18H20Cl2N2O2	C18H14Cl3NOS2	CI 7H15Cl2N3O
2,4-Dichloro-3-methyl-6-(4-methylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2- ethylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2- morpholin-4-yl-benzylamino)- phenol	2,4-Dichloro-3-methyl-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2,4-Dichloro-3-methyl-6-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol
TIN TO	F - 5	12 5 5	5 12 5 5	Z Z Z Z Z Z Z Z
503	504	505	206	507

367.4	404.5	296.8	350.7	335.0
367.09	404.29	296.20	350.17	334.60
Q	Ω	Ω	Ω	A
C12H10BrCl2NOS	C21H19Cl2NO3	C15H15Cl2NO	C15H12Cl2F3NO	C14H11Cl3FNO
2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro-3- methyl-phenol	2,4-Dichloro-6-[3-(4-methoxy-phenoxy)-benzylamino]-3-methyl-phenol	2,4-Dichloro-6-(3-methyl- benzylamino)-3-methyl-phenol	2,4-Dichloro-3-methyl-6-(3- trifluoromethyl-benzylamino)- phenol	2,4-Dichloro-3-methyl-6-(2-chloro-6-fluoro-benzylamino)-phenol
EZ ZO	TZ T	5 TZ	P CF3	5 -5
808	509	510	511	512

		<del></del>	
326.1	360.6	382.2	340.1
325.79	360.23	381.90	339.82
Q	D	D	Q
C19H16CINO2	C19H15ClZNO2	C23H24CINO2	C20H18CINO2
2-Chloro-6-(3-phenoxy-benzylamino)-phenol	2-Chloro-6-[3-(4-chloro-phenoxy)-benzylamino]-phenol	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-6-chloro-phenol	2-(3-Benzyloxy-benzylamino)-6- chloro-phenol
TZ TZ TO	5	5 Jo	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
513	514	515	516

	1	Т	T T	
340.1	284.0	280.2	294.3	319.1
339.82	283.75	279.79	293.81	318.80
Q	D	D	Q	. Д
C20H18CINO2	CI7H14CINO	C14H14CINOS	C15H16CINOS	C17H19CIN2O2
2-(2-Benzyloxy-benzylamino)-6- chloro-phenol	2-Chloro-6-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Chloro-6-(4-methylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-ethylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-morpholin-4-yl- benzylamino)-phenol
TZ TO	TZ 5	E TZ	20 12 20 30 12 30 30 30 30 30 30 30 30 30 30 30 30 30	
517	518	519	520	521

522	E S S S S S S S S S S S S S S S S S S S	2-Chloro-6-{[2-(4-chloro-phenylsulfanyl}-thiophen-3-ylmethyl]-amino}-phenol	C17H13Cl2NOS2	Q	382.33	382.6
523	TZ T	2-Chloro-6-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol	C16H14CIN3O	Q	299.75	300.2
524	TIN TO	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-6-chloro-phenol	C11H9BrCINOS	Д	318.62	319.5
525	5—0 5—0	2-Chloro-6-[3-(4-methoxy-phenoy)-benzylamino]-phenol	C20H18CINO3	Q	355.81	356.5
526	EZ E	2-Chloro-6-(3-methyl-benzylamino)-phenol	C14H14CINO	Q	247.72	248.5

.69 302.2	5.13 286.6	309.33 309.8	343.77 344.0	365.44 366.0
D 301.69	D 286.13	D 309	D 343	. D 365
C14H11CF3NO	C13H10Cl2FNO	C19H16FNO2	C19H15CIFNO2	C23H24FN02
2-Chloro-6-(3-trifluoromethyl-benzylamino)-phenol	2-Chloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	2-Fluoro-6-(3-phenoxy- benzylamino)-phenol	2-Fluoro-6-[3-(4-chloro-phenoxy)- benzylamino]-phenol	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-6-fluoro-phenol
CI OH H CF3	\$	172 4	5 L	
527	528	529	530	531

				11 mm
323.8	323.8	267.7	263.5	277.8
323.36	323.36	267.30	263.33	277.36
D	D	Q	Q	Q
C20H18FNO2	C20H18FNO2	C17H14FNO	C14H14FNOS	C15H16FNOS
2-(3-Benzyloxy-benzylamino)-6- fluoro-phenol	2-(2-Benzyloxy-benzylamino)-6- fluoro-phenol	2-Fluoro-6-[(naphthalen-1- yimethyl)-amino]-phenol	2-Fluoro-6-(4-methylsulfanyl- benzylamino)-phenol	2-Fluoro-6-(2-ethylsulfanyl- benzylamino)-phenol
\$ - \( \frac{1}{2} \)	TZ 5	₹	P IZ	EZ E
532	533	534	535	536

302.8	366.0	283.8	302.5	339.8
302.34	365.87	283.30	302.16	339.36
Д	Д	Q	Q	Q
C17H19FN2O2	C17H13CIFNOS2	C16H14FN3O	C11H9BrFNOS	C20H18FNO3
2-Fluoro-6-(2-morpholin-4-yl- benzylamino)-phenol	2-Fluoro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2-Fluoro-6-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-6-fluoro-phenol	2-Fluoro-6-[3-(4-methoxy-phenoxy)-benzylamino]-pheno
TZ E	TIN HO	Z Z TZ TO	IN TO TO	TZ TO
537	538	539	540	541

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542	E_F	2-Fluoro-6-(3-methyl-benzylamino)-phenol	C14H14FNO	Д	231.27	231.4
543	H H H H H H H H H H H H H H H H H H H	2-Fluoro-6-(3-trifluoromethyl-benzylamino)-phenol	C14H11F4NO	Q	285.24	285.5
544	5 - 5	2-Fluoro-6-(2-chloro-6-fluoro- benzylamino)-phenol	C13H10CIF2NO	D	269.67	270.1
545	5—————————————————————————————————————	2,3-Difluoro-6-(3-phenoxy- benzylamino)-phenol	C19H15F2NO2	D	327.32	327.6
546	-5 -5 -5	2,3-Difluoro-6-[3-(4-chloro- phenoxy)-benzylamino]-phenol	C19H14CIF2NO2	О	361.76	362.0

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383.8	341.7	341.7	285.6	281.6
383.43	341.35	341.35	285.29	281.32
D	Q		Q	Q
C23H23F2NO2	C20H17F2NO2	C20H17F2NO2	C17H13F2NO	C14H13F2NOS
2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-5,6-difluoro-phenol	2-(3-Benzyloxy-benzylamino)-5,6- C20H17F2NO2 difluoro-phenol	2-(2-Benzyloxy-benzylamino)-5,6- difluoro-phenol	2,3-Difluoro-6-[(naphthalen-1- ylmethyl)-amino]-phenol	2,3-Difluoro-6-(4-methylsulfanyl- benzylamino)-phenol
TZ E	5—————————————————————————————————————	₹	IZ E	TZ L
547	548	549	550	551

1	TZ E	2,3-Difluoro-6-(2-ethylsulfanyl- benzylamino)-phenol	CISHISFZNOS	Q	295.35	295.7
, , , , , , , , ,	TZ 5	2,3-Difluoro-6-(2-morpholin-4-yl- benzylamino)-phenol	C17H18F2N2O2	· Q	320.33	320.8
₹	5 5 122	2,3-Difluoro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	C17H12CIF2NOS2	Q	383.86	384.2
n - n	IZ TO	2,3-Difluoro-6-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol	C16H13F2N3O	Q	301.29	301.6
	E TE	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-5,6-difluoro- phenol	C11H8BrF2NOS	Д	320.15	320.4

357.6	249.6	303.7	288.1	. 347.0
357.35	249.26	303.23	287.66	346.23
D .	Д	Q	Ð	Ф
C20H17F2NO3	C14H13F2NO	C14H10F5NO	C13H9CIF3NO	C14H13Cl2NO3S
2,3-Difluoro-6-[3-(4-methoxy- phenoxy)-benzylamino]-phenol	2,3-Difluoro-6-(3-methyl- benzylamino)-phenol	2,3-Difluoro-6-(3-trifluoromethyl- benzylamino)-phenol	2,3-Difluoro-6-(2-chloro-6-fluoro-benzylamino)-phenol	N-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-C-phenyl- methanesulfonamide
TZ TO	TZ E	F. L.	\$	O HAN DO
557	558	559	999	561

295	CI OHO	Butane-1-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	C11H15Cl2N03S	д	312.21	312.1
563	D IN O H	Octane-1-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	C15HZ3Cl2NO3S	В	368.32	368.3
564	0 8 0 5	Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	C10H13Cl2NO3S	Ф	298.18	298.1
565	CI OH OH	N-(3,5-Dichloro-2-hydroxy- phenyl)-C-phenyl- methanesulfonamide	C13H11Cl2NO3S	В	332.20	332.4
999	D S OHO IS	Butane-1-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	C10H13Cl2NO3S	В	298.19	298.5

			P	
354.6	284.5	297.9	264.0	320.3
354.29	284.16	297.76	263.74	319.85
В	В	Ф	Ф	æ
C14H21CIZNO3S	C9H11Cl2NO3S	C13H12CINO3S	C10H14CINO3S	Ċ14HZ2CINO3S
Octane-1-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	N-(3-Chloro-2-hydroxy-phenyl)- C-phenyl-methanesulfonamide	Butane-1-sulfonic acid (3-chloro-2-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3-chloro- 2-hydroxy-phenyl)-amide
0 V O H	o do	O S OHO	C. OHO S. C.	TZ O O
267	568	569	570	571

572	C OID S	Propane-2-sulfonic acid (3-chloro-2-hydroxy-phenyl)-amide	C9H12CINO3S	В	249.71	250.4
573	HN-NHO H	N-(3-Fluoro-2-hydroxy-phenyl)-C- phenyl-methanesulfonamide	C13H12FNO3S	Ф	281.30	281.8
574		Butane-1-sulfonic acid (3-fluoro-2-hydroxy-phenyl)-amide	C10H14FNO3S	Д	247.29	247.8
575	IN OF STATE	Octane-1-sulfonic acid (3-fluoro-2-hydroxy-phenyl)-amide	C14H22FNO3S	Д	303.39	303.8
576	O HN HO	Propane-2-sulfonic acid (3-fluoro- 2-hydroxy-phenyl)-amide	C9H12FNO3S	щ	233.26	233.7
577	NH OHO J	N-(3,4-Diffuoro-2-hydroxy- phenyl)-C-phenyl- methanesulfonamide	C13H11F2NO3S	Ф	299.29	300.8

265.7	321.8	251.6	320.2	306.4
265.28	321.38	251.25	320.22	306.18
В	В	В	F, G, H	В, С, Н
C10H13F2NO3S	C14H21F2NO3S	C9H11F2NO3S	C14H19Cl2NO3	C13H17Cl2NO3
Butane-1-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-carbamic acid hexyl ester	(3,5-Dichloro-2-hydroxy-phenyl)- carbamic acid hexyl ester
HN HO	TZ OF	O S HN HO	20 P P P P P P P P P P P P P P P P P P P	HA CI
578	579	580	581	582

272.1	. 255.6	334.5	273.6	377.1
271.74	255.29	334.18	273.28	377.26
F, G, H	F, G, H	F, G, H	F, G, H	4
C13H18CINO3	C13H18FNO3	C13H17BrFNO3	C13H17F2NO3	C16H22Cl2N2O4
(3-Chloro-2-hydroxy-phenyl)- carbamic acid hexyl ester	(3-Fluoro-2-hydroxy-phenyl)- carbamic acid hexyl ester	(5-Bromo-3-fluoro-2-hydroxy- phenyl)-carbamic acid hexyl ester	(3,4-Difluoro-2-hydroxy-phenyl)- carbamic acid hexyl ester	2-[3-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester
DE OF	₽ OF OF	OH OH OH	u y y y y y y y y y y y y y y y y y y y	
583	584	585	586	587

-	CI C	2-[3-(3,5-Dichloro-2-hydroxy-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20Cl2N2O4	ď	363.24	363.6
	TZ O	2-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	C15HZ1CINZ04	∢	328.79	329.1
	TZ O	2-[3-(3-Fluoro-2-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	C15H21FN2O4	<b>∀</b>	312.34	312.8
	IZ O	2-[3-(3,4-Difluoro-2-hydroxy-4-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20F2N2O4	<b>∀</b>	330.33	330.8
	IZ O	2-[3-(5-Bromo-3-fluoro-2-hydroxy-4-methyl-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20BrFN2O4	4	391.23	391.6

411.1	397.6	363.0	346.7
411.28	397.25	362.81	346.35
Ą	<b>∀</b>	<b>A</b>	¥
C19H20Cl2N2O4	C18H18CIZN2O4	C18H19CINZO4	C18H19FN2O4
2-[3-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	2-[3-(3,5-Dichloro-2-hydroxy- phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	2-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3-Fluoro-2-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester
TZ O TZ	TZ O TZ O	E S	TZ TZ
593	594	595	969

. ∞	. 9	٧.
364.8	425.6	332.5
364.34	425.25	332.27
∢	<b>∀</b>	ς Έ
C18H18F2N2O4	C18H18BrFN2O4	C16H23CI2NO2
2-[3-(3,4-Difluoro-2-hydroxy- phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	2-[3-(5-Bromo-3-fluoro-2- hydroxy-phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide
TZ O	TZ O	2 12 2 3
297	598	299

				4162			
	Structure	Chemical name	Formula	Synthesis	MolWeight	MS data	
009	TZ TO TO	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	C15H21C12NO2	C, B	318.24	318.5	
601	TZ 5	3,5,5-Trimethyl-hexanoic acid (3-chloro-2-hydroxy-phenyl)-amide	C15H22CINO2	C, E	283.79	284.0	
602	5— S—	3,5,5-Trimethyl-hexanoic acid (3-fluoro-2-hydroxy-phenyl)-amide	C15H21FN02	හි ·	267.34	267.7	
603	TZ TZ	3,5,5-Trimethyl-hexanoic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	C15H21F2NO2	я У	285.33	285.7	

	13	
346.5	383.4	439.8
346.24	382.88	438.99
С, Е	J followed by A	J followed by
C15H21BrFNO2	C18H27CIN4O3	C22H35CIN4O3
3,5,5-Trimethyl-hexanoic acid (5-bromo-3-fluoro-2-hydroxy-phenyl)-amide	1-tert-Butyl-3-[3-chloro-5-(3- cyclohexyl-ureido)-2-hydroxy- phenyl]-urea	1-[3-Chloro-5-(3-cyclohexyl- ureido)-2-hydroxy-phenyl]-3- (1,1,3,3-tetramethyl-butyl)-urea
12 5	→ ST	NI ON SI
<b>260</b>	909	909

517.4	450.9	426.4
516.48	449.97	426.31
J followed by D	J followed by D	J followed by D
C26H27Cl2N3O2S	C26H28CIN3O2	C20H22Cl2FN3O2
1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl}-benzylamino]-4-hydroxy-phenyl}-3-cyclohexylurea	1-{3-[(Biphenyl-2-ylmethyl)- amino]-5-chloro-4-hydroxy- phenyl}-3-cyclohexyl-urea	1-[3-Chloro-5-(2-chloro-6-fluoro-benzylamino)-4-hydroxy-phenyl]-3-cyclohexyl-urea
S S S S S S S S S S S S S S S S S S S	T T TO	ZI O O O
209	809	609

404.9	406.8	406.8
404.89	405.88	405.88
J followed by A	J followed by G	J followed by G
C20H25CIN4O3	C20H24CIN3O4	C20H24CIN3O4
1-tert-Butyl-3-[3-chloro-2- hydroxy-5-(3-phenethyl-ureido)- phenyl]-urea	[3-Chloro-2-hydroxy-5-(3- phenethyl-ureido)-phenyl]- carbamic acid isobutyl ester	[3-Chloro-2-hydroxy-5-(3-phenethyl-ureido)-phenyl]-carbamic acid sec-butyl ester
TZ NH	PO NH NH	HO NH H
610	611	612

401.9	415.9	413.8
401.89	415.92	412.95
J followed by C	J followed by C	I followed by A
C21H24CIN3O3	C22H26CIN3O3	C20H33CiN4O3
Cyclopentanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenethylureido)-phenyl]-amide	Cyclohexanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenethylureido)-phenyl]-amide	1-tert-Butyl-3-{3-chloro-2- hydroxy-5-[3-(1,1,3,3-tetramethyl- butyl)-ureido]-phenyl}-urea
	TZ O NH	TZ O NT
613	614	615

413.8	414.1	381.9
413.94	413.94	381.90
J followed by G	J followed by G	J followed by C
C20H32CIN3O4	C20H32CIN3O4	C19H28CIN3O3
{3-Chloro-2-hydroxy-5-[3- (1,1,3,3-tetramethyl-butyl)- ureido]-phenyl}-carbamic acid isobutyl ester	{3-Chloro-2-hydroxy-5-[3- (1,1,3,3-tetramethyl-butyl)- ureido]-phenyl}-carbamic acid sec- butyl ester	Cyclopropanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide
D NH H	HO NE	TZ O NH
. 616	617	618

395.9	410.1	424.0
395.92	409.95	423.98
J followed by C	J followed by C	J followed by
C20H30CIN3O3	C21H32CIN3O3	C22H34CIN3O3
Cyclobutanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide	Cyclopentanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide	Cyclohexanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide
D NH	D NH	TZ O NH
619	620	621

389.9	390.8	390.8
389.88	390.86	390.86
L followed by A	L followed by G	L followed by G
C20H24CIN3O3	C20H23CIN2O4	C20H23CIN2O4
N-[3-(3-text-Butyl-ureido)-5- chloro-4-hydroxy-phenyl]-3- phenyl-propionamide	[3-Chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-carbamic acid isobutyl ester	[3-Chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-carbamic acid sec-butyl ester
D IN O O O	E N	TZ O
	623	624

<b>—</b>		
358.9	373.8	386.8
358.82	372.85	386.87
L followed by C	L followed by C	L followed by C
C19H19CIN2O3	C20H21CIN2O3	C21HZ3CINZO3
Cyclopropanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide	Cyclobutanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide	Cyclopentanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide
E	5 - Z	TZ O TZ
625	979	627

401.8	319.7	342.3
400.90	319.25	341.85
L followed by C	I	Q
C22H24CIN2O3	C13H16Cl2N2OS	C19H16CINOS
Cyclohexanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide	1-Cyclopentyl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-thiourea	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-phenol
P N	IZ S	z zz s
	629	930

525.1	539.1	545.5
524.46	538.49	544.88
J followed by D	J followed by D	J followed by D
CZ7HZ3ClZN3O2S	C28H25CI2N3O2S	C26H20Cl3N3O2S
1-Benzyl-3-{3-chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-urea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-phenethyl-urea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-(4-chloro-phenyl)-urea
\$\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\		NI N
5	5	5
631	632	633

376.1	382.2	376.1
375.9	381.90	375.9
J followed by B	J followed by	K followed by A
C15H22CIN3O4S	C19H28CIN3O3	C18H18CIN3O2S
Ethanesulfonic acid [3-chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-amide	N-[3-Chloro-5-(3-cyclohexyl- ureido)-2-hydroxy-phenyl]-3,3- dimethyl-butyramide	1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-tert-butyl-urea
634	635	636

410.1	424.1	378.1
409.9	423.9	377.9
K followed by A	K followed by A	K followed by
C21H16CIN3O2S	C22H18CIN3O2S	C17H16CIN3OS2
1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-benzyl-urea	1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-phenethyl-urea	1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-isopropyl- thiourea
12 0 12 0		
637	638	639

392.1	417.2	409.2	256.9
391.9	417.0	408.9	263.31
K followed by I	K followed by C	K followed by C	A
C18H18CIN3OS2	C22H25CIN2O2S	C22H17CIN2O2S	C13H20N2O2
1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-tert-butyl- thiourea	3,5,5-Trimethyl-hexanoic acid (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-amide	N-(5-Benzothiazol-2-yl-3-chloro- 2-hydroxy-phenyl)-3-phenyl- propionamide	1-(2-Hydroxy-4-methyl-phenyl)-3- pentyl-urea
	HO NH	TN. Ho	FZ O
640	641	642	643

	,			
372.6	358.5	272.6	258.4	225.7
372.24	358.22	272.13	258.10	225.19
CorE	CorE	Q	Q.	۵
C20H15CI2NO2	C20H15Cl2NO2	C12H11CI2NO2	C11H9Cl2NO2	C11H9F2NO2
Biphenyl-4-carboxylic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	Biphenyl-4-carboxylic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	2,4-Dichloro-6-[(furan-2- ylmethyl)-amino]-3-methyl-phenol	2,4-Dichloro-6-[(furan-2- ylmethyl)-amino]-phenol	2,3-Difluoro-6-[(furan-2- ylmethyl)-amino]-phenol
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	TZ B	TZ TZ		TN TO THE TOTAL TO
4	645	949	647	648

350.5	336.5	303.6	580.9
350.16	336.14	303.23	580.31
D	D	D	J followed by D
CISH12CIZF3NO	C14H10Cl2F3NO	C14H10F5NO	C25H18Cl4N4O2S
2,4-Dichloro-3-methyl-6-(2- trifluoromethyl-benzylamino)- phenol	2,4-Dichloro-6-(2-trifluoromethyl-benzylamino)-phenol	2,3-Difluoro-6-(2-trifluoromethyl-benzylamino)-phenol	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-(2,6-dichloro-pyridin-4-yl)-urea
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	12 E	
649	059	651	652

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404.6	520.1	282.7	379.9
403.95	519.44	282.17	379.24
K followed by I	J followed by D	Q	<b>⋖</b>
C19H18CIN3OS2	C24H24C12N4O3S	C14H13Cl2NO	C17H16CI2N4O2
1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-cyclopentyl- thiourea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-morpholin-4-yl-urea	6-Benzylamino-2,4-dichloro-3- methyl-phenol	1-[2-(1H-Benzoimidazol-2-yl)- ethyl]-3-(3,5-dichloro-2-hydroxy- 4-methyl-phenyl)-urea
TZ S S S S S S S S S S S S S S S S S S S	D D D D D D D D D D D D D D D D D D D	5—5 5—7 5—7 5—7 5—7 5—7 5—7 5—7 5—7 5—7	D HO D
653	654	655	959

404.6	384.4	398.2	418.9
403.95	383.89	397.92	418.34
K followed by I	Q	Ω	.Ω
C19H18CIN3OS2	C21H18CINO2S	C22HZ0CINO2S	C21H17Cl2NO2S
1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-cyclopentyl-thiourea	1-[5-Chloro-2-hydroxy-3-(2-phenylsulfanyl-benzylamino)-phenyl]-ethanone	1-[5-Chloro-2-hydroxy-3-(2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone	1-{5-Chloro-3-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone
	5—0—0	5—0= 5—0=	5 5 5 5
657	829	629	099

429.3	414.3	418.9	418.8	453.2
428.89	413.92	418.34	418.34	452.78
D	D	D	Ω.	Q
C21H17CIN2O4S	C22H20CINO3S	C21H17Cl2NO2S	C21H17CI2NO2S	C21H16Cl3NO2S
1-{5-Chioro-2-hydroxy-3-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenyl}-ethanone	1-{5-Chloro-2-hydroxy-3-[2-(4-methoxy-phenylsulfanyl)-benzylamino}-phenyl}-ethanone	1-{5-Chloro-3-[2-(2-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{5-Chloro-3-[2-(3-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{5-Chloro-3-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone
TZ TO TO	1Z 5	5 -5 o -	5 	5 5 5 5 6 0 0
661	662	699	664	\$99

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441.4	435.3	463.9	443.3
440.94	434.94	463.33	442.92
D	Ω.	Q	Q
C23H21CIN2O3S	C24H19CIN2O2S	C21H16Cl2N2O4S	C22H19CIN2O4S
N-(4-{2-[(3-Acetyl-5-chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	1-{5-Chloro-2-hydroxy-3-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenyl}-ethanone	1-{5-Chloro-3-{2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-2-hydroxy-phenyl}-ethanone	1-[5-Chloro-2-hydroxy-3-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone
5 TZ TÖ	TZ TO O	0 - 0 - 0	\$ 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
999	<i>L</i> 99	899	699

C21H18CI2N2O2S
C21H17Cl2NO4S
C19H16CINO2S
1,6-Di-(3,5-Dichloro-2-hydroxy-4- C22H26CI4N4O4 methyl-phenyl)-3-hexyl-urea
3-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-propionic acid ethyl ester

675	IN OF	1-(3-Chloro-4-hydroxy-phenyl)-3- pentyl-urea	C12H17CIN2O2	A	256.73	256.9
929	IZ O	1-Benzyl-3-(3-chloro-4-hydroxy-phenyl)-urea	C14H13CIN2O2	Ą	276.72	276.9
21.9	EN O	1-(3-Chloro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	C15H15CIN2O2	٧	290.74	290.9
829	IZ O	1-(3-Chloro-4-hydroxy-phenyl)-3- phenethyl-urea	C15H15CIN2O2	¥	290.75	291.2
629	DE STEEL STE	1-(3-Chloro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	C15H23CIN2O2	Ä	298.81	299.4
089	IZ D D D D D D D	1-tert-Butyl-3-(3-chloro-4- hydroxy-phenyl)-urea	C11H15CIN2O2	₽	242.70	243.0

170

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283.1	345.0	331.9	297.7	331.0	269.1
282.77	344.72	331.59	297.14	330.69	268.74
∢	æ	¥	А	. <b>∢</b>	4
C14H19CIN2O2	C15H12CIF3N2O2	C13H9Cl3N2O2	C13H10Cl2N2O2	C14H10CIF3N2O2	C13H17CIN2O2
1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Chloro-3-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexyl-urea
IZ OF	IZ O	D TZ OH	HZ OH	HN O IN O OF O	IZ O H
681	682	683	684	589	989

			T		
346.9	287.9	306.9	276.9	292.9	290.9
346.69	287.70	306.70	276.72	292.72	290.75
Ą	<b>∀</b>	Ą	A	<b>V</b> .	∢
C14H10CIF3NZO3	C14H10CIN302	C14H11CIN2O4	C14H13CIN2O2	C14H13CIN2O3	C15H15CIN2O2
1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3- chloro-4-hydroxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- o-tolyl-urea	1-(3-Chioro-4-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea
HO HOOF3	TZ O TZ	IZ O	TZ O	HO N N N N N N N N N N N N N N N N N N N	IZ O
289	889	689	069	691	692

353.2	313.1	321.4	354.9	263.2
352.77	312.75	320.82	354.79	262.70
V V	¥	∢	A	. ч
C16H17CIN2O5	C17H13CIN2O2	C17H21CIN2O2	C19H15CINZO3	C13H11CIN202
1-(3-Chloro-4-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3-chloro-4- hydroxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenyl-urea
N N O O O O O O O O O O O O O O O O O O	DHO HZ		HN OOH	IZ O
693	694	695	969	269

Henry 1-3-(3,5-Dichloro-4-hydroxy-  henry 1-(3,5-Dichloro-4-hydroxy-  henry 1-3-5-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  1-(3,5-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  1-(3,5-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  1-(3,5-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  henry 1-3-2-Dichloro-4-hydroxy-  henry 1-3-2-Dichloro-4-hydroxy-  henry 1-3-2-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  henry 1-3-2-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-  henry 1-3-3-peramethy 1-  henry 1-3-3-peramethy 1-  henry 1-3-2-Dichloro-4-hydroxy-  henry 1-3-3-peramethy 1-3-6-peramethy 1-3-5-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-3-6-peramethy 1-							
1-(3,5-Dichloro-4-hydroxy-   C12H16C12N2O2   A   291.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17   201.17		TZ O	oxy-	C12H14Cl2N2O4	¥	321.16	321.9
1-Benzyl-3-(3,5-dichloro-4-   C14H12C12N2O2   A   311.16		IZ DIZ	roxy-	C12H16CI2N2O2	<b>∢</b>	291.17	292.0
CI SH14CI2NZOZ A 325.19  CI SH14CI2NZOZ A 325.19  phenyl)-3-(2-methyl-benzyl)-urea  CI SH14CI2NZOZ A 325.19  phenyl)-3-phenethyl-wea  CI SH14CI2NZOZ A 325.19  phenyl)-3-phenethyl-wea  CI SH14CI2NZOZ A 333.25  phenyl)-3-(1,1,3,3-tertamethyl- C15H22CI2NZOZ A 333.25		IZ DO	1-Benzyl-3-(3,5-dichloro-4- hydroxy-phenyl)-urea	C14H12Cl2N2O2	¥	311.16	312.0
CI MAN HOLISTON A 325.19  CISH14CI2N202 A 325.19  CISH14CI2N202 A 333.25  Phenyl)-3-phenethyl-urea  CISH14CI2N202 A 333.25  Phenyl)-3-phenethyl-urea  CISH14CI2N202 A 333.25  Phenyl)-urea		_5	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	C15H14Cl2N2O2	∢	325.19	325.9
CI SH22CI2N202 A 333.25 phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea		TZ -ō	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenethyl-urea	C15H14Cl2N2O2	Ä	325.19	325.9
	1	IZ DIZ	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea	C15H22Cl2N2O2	Ą	333.25	334.0

11H14CL	L-tert-butyt-5-(5,5-mcmono-+- hydroxy-phenyl)-urea
14H18Cl2N	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-cyclohexylmethyl-wea
15H11Cl2F	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea
)13H8Cl4N2O	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)- urea
213H9Cl3N2C	1-(3,5-Dichloro-4-hydroxy-phenyl)-urea
C14H9CIZF3N	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-urea

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304.0	381.8	322.9	341.7	311.8	327.5
303.18	381.13	322.15	341.15	311.16	327.16
¥	∢	¥	¥	Α .	Ą
C13H16Cl2N2O2	C14H9Cl2F3N2O3	C14H9ClZN3O2	C14H10Cl2N2O4	C14H12Cl2N2O2	C14H12Cl2N2O3
1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5- dichloro-4-hydroxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-o-tolyl-urea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3-methoxy-phenyl)- urea
IN OH	HO IN OOF	ZZ O TZ	TZ O TZ	IZ O T	HO HO WAS
710	711	712	713	714	715

325.6	387.6	347.6	355.7	389.6
325.19	387.21	347.20	355.26	389.23
A	A	<b>∀</b>	¥	A
C15H14Cl2N2O2	C16H17CI2N2O5	C17H12CI2N2O2	C17HZ0Ci2NZO2	C19H14Cl2N2O3
1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(2,6-dimethyl-phenyl)-	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-dichloro-4-hydroxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea
TZ OF	C C C C C C C C C C C C C C C C C C C	IZ DEO	D TZ O	N O OH
716	717	718	719	720

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297.7	297.8	267.9	287.9	301.8	301.8	309.8
297.14	297.26	267.28	287.27	301.30	301.30	309.36
V	A	Ą	¥	¥	. <b>4</b>	Ą
C13H10Cl2N2O2	C12H15N3O6	C12H17N3O4	C14H13N3O4	C15H15N3O4	C15H15N3O4	C15H23N3O4
1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-urea	3-[3-(4-Hydroxy-3-nitro-phenyl)- ureido]-propionic acid ethyl ester	1-(4-Hydroxy-3-nitro-phenyl)-3- pentyl-urea	1-Benzyl-3-(4-hydroxy-3-nitro- phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-methyl-benzyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenethyl-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea
IZ O T	IN OH	NY OH	IN O	IN OO IN		IZ OH
721	722	723	724	725	726	727

253.8	293.9	355.8	342.7	308.4	341.8	279.8
253.25	293.32	355.27	342.13	307.69	341.24	279.29
¥.	A	∢	V	A	. <b>4</b>	A
C11H15N3O4	C14H19N3O4	C15H12F3N3O4	C13H9C12N3O4	C13H10CIN3O4	C14H10F3N3O4	C13H17N3O4
1-tert-Butyl-3-(4-hydroxy-3-nitro-phenyl)-urea	1-Cyclohexylmethyl-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3,5-Dichloro-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Chloro-phenyl)-3-(4-hydroxy- 3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-Cyclohexyl-3-(4-hydroxy-3- nitro-phenyl)-urea
IN NO S	IN O	O ₂ N H N O O O O O O O O O O O O O O O O O	IN OH OH	IN O	IZ O IZ	IN OH
728	729	730	731	732	733	734

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357.9	298.9	317.9	287.9	303.8	301.9	364.0
357.24	298.25	317.25	287.27	303.27	301.30	363.32
Ą	∢	<b>∀</b>	¥	¥	₩ .	<b>V</b>
C14H10F3N3O5	C14H10N4O4	C14H11N3O6	C14H13N3O4	C14H13N3O5	C15H15N3O4	C16H17N3O7
1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(4-Cyano-phenyl)-3-(4-hydroxy- 3-nitro-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3-o- tolyl-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (3-methoxy-phenyl)-urea	1-(2,6-Dimethyl-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea
O ₂ N H H N OCF ₃	O ₂ N N N O N O N O N O N O N O N O N O N O	O _N N N N N N N N N N N N N N N N N N N N	HZ O OH	O N O N O N O O O O O O O O O O O O O O	HZ OH	O ₂ N H H OMe
735	736	737	738	739	740	741

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323.9	331.9	366.0	273.9	270.6	240.5	260.8
323.30	331.37	365.34	273.24	270.26	240.27	260.26
∢	¥	Ą	¥	¥	. <b>«</b>	ď
C17H13N3O4	C17H21N3O4	C19H15N3O5	C13H11N3O4	C12H15FN2O4	C12H17FN2O2	C14H13FN2O2
1-(4-Hydroxy-3-nitro-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(4-hydroxy- 3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenyl-urea	3-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(3-Fluoro-4-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-fluoro-4-hydroxy- phenyl)-urea
N ₂ O ₂ N H O ₂ O ₂ O ₃ H	HZ OH	IZ	N O N O O O O O O O O O O O O O O O O O	TZ OH	IN OH	IZ O
742	743	744	745	746	747	748

	IZ	1-(3-Fluoro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	C15H15FN2O2	Ą	274.29	274.9
2 L/	IZ O IZ	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenethyl-urca	CI5H15FN2O2	A	274.29	274.6
		1-(3-Fluoro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	C15H23FN2O2	A	282.35	282.9
		1-tert-Butyl-3-(3-fluoro-4-hydroxy-phenyl)-urea	C11H15FN2O2	∢	226.25	226.5
]	IN O	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexylmethyl-urea	C14H19FN2O2	¥	266.31	266.7
[	TX TX	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	C15H12F4N2O2	A	328.26	328.4
2		1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	C13H9ClZFN2O2	<b>∀</b>	315.13	315.5
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281.1	314.6	252.6	330.5	271.5	290.7	260.5	276.5
280.68	314.24	252.28	330.23	271.25	290.25	260.26	276.26
A	A	Ą	¥	¥	A	¥	A
C13H10CIFN2O2	C14H10F4N2O2	C13H17FN2O2	C14H10FF3N2O3	C14H10FN3O2	C14H11FN2O4	C14H13FN2O2	C14H13FN2O3
1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexyl-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3- fluoro-4-hydroxy-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- o-tolyl-urea	1-(3-Fluoro 4-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea
IN O	HZ POP	IZ O	HOOF!	TZo	IZ STE		HO LA COMB
756	757	758	759	760	761	762	763

762	IZ O	1-(3-Fluoro-4-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	C15H15FN2O2	¥	274.29	274.7
765	HO HO OME	1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	C16H17FN2OS	¥	336.31	336.6
992	IZ O	1-(3-Fluoro-4-hydroxy-phenyl)-3- naphthalen-1-yl-urea	C17H13FN2O2	∢	296.3	296.6
191	TZ Q	1-Adamantan-1-yl-3-(3-fluoro-4- hydroxy-phenyl)-urea	C17H21FN2O2	∢ .	304.36	304.6
892	N N N N N N N N N N N N N N N N N N N	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	C19H15FN2O3	A	338.33	338.6
769	IZ O IZ O	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenyl-urea	C13H11FN2O2	A	246.24	246.5

OH H H A 1-(2,4-Dihydroxy-phenyl)-3- C12H16N2O3 A 238.28  HO OH H H A 1-(2,4-Dihydroxy-phenyl)-3- C12H18N2O3 A 238.28  HO OH H H A 1-(2,4-Dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3- C15H16N2O3 A 272.30  HO OH H H A 1-(2,4-Dihydroxy-phenyl)-3- C15H16N2O3 A 270.30  HO OH H H A 1-(2,4-Dihydroxy-phenyl)-3- C15H16N2O3 A 280.36  HO OH H H A 1-(2,4-Dihydroxy-phenyl)-3- C15H16N2O3 A 280.36  HO OH H H A 1-tert-Butyl-butyl)-urea  OH H H A 1-tert-Butyl-3-(2,4-dihydroxy-phenyl)-3- C11H16N2O3 A 224.26  Dhenyl)-urea							
OH H H H LOCA-Dihydroxy-phenyl)-3- C12H18N2O3 A pentyl-urea pentyl-urea phenyl)-urea phenyl)-urea henyl)-urea methyl-benzyl)-urea methyl-benzyl)-urea phenyl)-3-(2-Dihydroxy-phenyl)-3- C15H16N2O3 A phenethyl-urea phenyl)-3- C15H16N2O3 A phenethyl-urea (1,1,3,3-tetramethyl-butyl)-urea (1,1,3,3-tetramethyl-butyl)-urea phenyl)-3- C15H16N2O3 A phenyl)-urea phenyl)-urea	Ā	HZ O HZ	3-[3-(2,4-Dihydroxy-phenyl)- ureido]-propionic acid ethyl ester	C12H16N2O5	Ą	268.27	268.7
OH H H H L-2.4-Dihydroxy-phenyl)-3-(2.4-dihydroxy-phenyl)-3-(2.5H16N2O3 A methyl-benzyl)-urea  OH H H H L-(2.4-Dihydroxy-phenyl)-3- OH H H L-(2.4-Dihydroxy-phenyl)-3- OH H H L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Dihydroxy-phenyl)-urea  OH L-(2.4-Dihydroxy-phenyl)-3- OH L-(2.4-Di	ř	£	1-(2,4-Dihydroxy-phenyl)-3- pentyl-urea	C12H18N2O3	∢	238.28	238.6
OH H H H L 1-(2,4-Dihydroxy-phenyl)-3-(2-C15H16N2O3 A methyl-benzyl)-urea  OH H H H L 1-(2,4-Dihydroxy-phenyl)-3-C15H16N2O3 A phenethyl-wrea  OH H H H L 1-(2,4-Dihydroxy-phenyl)-3-C15H24N2O3 A (1,13,3-tetramethyl-butyl)-wrea  OH H H H L 1-tert-Butyl-3-(2,4-dihydroxy-phenyl)-3-C11H16N2O3 A phenyl)-wrea		Į Į	1-Benzyl-3-(2,4-dihydroxy- phenyl)-urea	C14H14N2O3	∢	258.27	258.6
OH H H T 1-(2,4-Dihydroxy-phenyl)-3- C15H16N2O3 A phenethyl-urea phenethyl-butyl)-3- C15H24N2O3 A (1,1,3,3-tetramethyl-butyl)-urea (1,1,3,3-tetramethyl-butyl)-urea phenyl)-urea phenyl)-urea		F TZ	1-(2,4-Dihydroxy-phenyl)-3-(2- methyl-benzyl)-urea	C15H16N2O3	∢	272.30	272.5
OH H H Text-Butyl-3-C15H24N2O3 A  1-(2,4-Dihydroxy-phenyl)-3-C15H24N2O3 A  (1,1,3,3-tetramethyl-butyl)-urea phenyl)-urea phenyl)-urea		£	1-(2,4-Dihydroxy-phenyl)-3- phenethyl-urea	C15H16N2O3	¥	272.30	272.5
OH H H 1-tert-Butyl-3-(2,4-dihydroxy- C11H16N2O3 A phenyl)-urea		₹ Tz 0	1-(2,4-Dihydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	C15H24N2O3	. <b>4</b>	280.36	280.7
) OH		TZ O	1-tert-Butyl-3-(2,4-dihydroxy- phenyl)-urea	C11H16N2O3	¥	224.26	224.8

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777  1-Cyclohexylmethyl-3-(2,4- C14)  1-Cyclohexylmethyl-3-(2,4- C14)  1-(2,4-Dihydroxy-phenyl)-3-(4- C15)  1-(2,4-Dihydroxy-phenyl)-3-(4- C15)  1-(3,5-Dichloro-phenyl)-3-(2,4- C13)  1-(4-Chloro-phenyl)-urea dihydroxy-phenyl)-urea dihydroxy-phenyl	-						
OH H H H CI (2,4-Dihydroxy-phenyl)-3-(4-trifluoromethyl-benzyl)-urea (4,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-urea (4,4-dihydroxy-phenyl)-urea (	777	£	1-Cyclohexylmethyl-3-(2,4- dihydroxy-phenyl)-urea	C14H20N2O3	A	264.32	264.7
OH HO CI 1-(3,5-Dichloro-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-3-(4-trifluoromethyl-phenyl)-urea	778	TIN TO TIN	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-benzyl)-urea	C15H13F3N2O3	¥	326.27	326.8
HO OH H H I - (4-Chloro-phenyl)-3-(2,4-dihydroxy-phenyl)-urea HO HO CF ₃ HO CF ₃ 1-(4-Chloro-phenyl)-3-(2,4-dihydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-urea	677	IZ DEO	1-(3,5-Dichloro-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	C13H10Cl2N2O3	V	313.14	313.7
1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-phenyl)-urea	780	EZ E	1-(4-Chloro-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	C13H11CINZO3	¥	278.69	279.2
	781	IZ Ā	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-phenyl)-urea	C14H11F3N2O3	<b>V</b>	312.24	312.8
782 HO HO Dhenyl)-urea C1:	782	IZ D=0	1-Cyclohexyl-3-(2,4-dihydroxy- phenyl)-urea	C13H18N2O3	A	250.29	250.8

328.7	269.8	288.9	258.7	274.8	272.9	
328.24	269.26	288.26	258.27	274.27	272.30	
∢	∢	∢	ď	<b>V</b>	. <b>«</b>	
C14H11F3N2O4	C14H11N3O3	C14H12N2O5	C14H14N2O3	C14H14N2O4	C15H16N2O3	
1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethoxy-phenyl)-urea	1-(4-Cyano-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(2,4- dihydroxy-phenyl)-urea	1-(2,4-Dihydroxy-phenyl)-3-0- tolyl-urea	1-(2,4-Dihydroxy-phenyl)-3-(3- methoxy-phenyl)-urea	1-(2,4-Dihydroxy-phenyl)-3-(2,6- dimethyl-phenyl)-urea	
HOOF ₂	F S	HO OH	TZ O TZ	HO NO	IZ O	H H H
783	784	785	786	787	788	

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294.9	302.8	336.9	244.7	410.4	380.5
294.30	302.37	336.34	244.25	410.06	380.08
¥	∢	¥	ď	Ψ.	A
C17H14N2O3	C17H22N2O3	C19H16N2O4	C13H12N2O3	acid C12H14Br2N2O4	C12H16Br2N2O2
1-(2,4-Dihydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(2,4- dihydroxy-phenyl)-urea	1-(2,4-Dihydroxy-phenyl)-3-(4- phenoxy-phenyl)-urea	1-(2,4-Dihydroxy-phenyl)-3- phenyl-urea	3-[3-(3,5-Dibromo-4-hydroxy-phenyl)-ureido]-propionic acid ethyl ester	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-pentyl-urea
TIN OF	5—————————————————————————————————————	12 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	\$ 12 0 E	N N O H	TN O TN O
790	791	792	793	794	795

400.4	414.5	414.4	422.5	366.4	406.5
400.07	414.09	414.09	422.16	366.05	406.11
Ą	<b>∀</b>	¥	A	Ā	¥
C14H12Br2N2O2	C15H14Br2N2O2	C15H14Br2N2O2	C15H22Br2N2O2	C11H14Br2N2O2	C14H18Br2N2O2
1-Benzyl-3-(3,5-Dibromo-4- hydroxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3,5-dibromo-4- hydroxy-phenyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexylmethyl-urea
IZ OF	IN OH	IN OH	IN OH	TZ O TZ	TX O
796	797	798	799	008	801

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468.4	455.4	420.7	454.3	392.5	470.3
468.06	454.93	420.48	454.04	392.09	470.04
4	∢	¥	¥	¥	4
C15H11Br2F3N2O2	C13H8Br2Cl2N2O2	C13H9Br2CIN2O2	C14H9Br2F3N2O2	C13H16Br2N2O2	C14H9Br2F3N2O3
1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea
HO HO OF 3	TN O	IN OH	HO NH CFs	N O H	HO NH
802	803	804	805	908	807

808	HO NO	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	C14H9Br2N3O2	Ą	411.05	411.5
809	HO H	1-Benzo[1,3]dioxol-5-yl-3-(3,5- dibromo-4-hydroxy-phenyl)-urea	C14H10Br2N2O4	¥	430.05	430.3
810	HO NH OH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-o-tolyl-urea	C14H12Br2N2O2	<b>∢</b>	400.07	400.4
811	HO N N N N N N N N N N N N N N N N N N N	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	C14H12Br2N2O3	¥	416.06	416.3
812	IN OH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	C15H14Br2N2O2	Ψ.	414.09	414.5
813	Br OMB	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(3,4,5-trimethoxy- phenyl)-urea	C16H17Br2N2O5	A	476.12	476.4

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436.4	444.2	478.3	386.2	288.9
436.10	444.16	478.13	386.04	288.25
Ą	<b>∀</b>	¥	A	. <b>V</b>
C17H12Br2N2O2	C17H20Br2N2O2	C19H14Br2N2O3	C13H10Br2N2O2	acid C12H14F2N2O4
1-(3,5-Dibromo-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-dibromo- 4-hydroxy-phenyl)-urea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenyl-urea	3-[3-(3,5-Difluoro-4-hydroxy- phenyl)-ureido]-propionic acid ethyl ester
TN O H	TN OH	HO H	TZ O TZ	IX O IX O IX
814	815	816	817	818

819	TN OF	I-(3,5-Difluoro-4-hydroxy- phenyl)-3-pentyl-urea	C12H16F2N2O2	Ą	258.26	258.9
820	IN OH	1-Benzyl-3-(3,5-difluoro-4- hydroxy-phenyl)-urea	C14H12F2N2O2	∢	278.25	278.8
821	HZ OH	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	C15H14F2N2O2	<b>∀</b>	292.28	292.9
822	TZ OH	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenethyl-urea	C15H14F2N2O2	4	292.28	292.9
823	TZ O LX	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	C15H22F2N2O2	· <b>V</b>	300.34	300.5
824	IZ OF U	1-tert-Butyl-3-(3,5-difluoro-4- hydroxy-phenyl)-urea	C11H14F2N2O2	<b>∀</b>	244.24	244.3

284.6	346.5	333.3	298.9	332.7	270.7
284.30	346.25	333.12	298.67	332.23	270.28
¥	Ą	∢	4	· <b>4</b>	A
C14H18F2N2O2	C15H11F5N2O2	C13H8Cl2F2N2O2	C13H9CIF2N2O2	C14H9F5N2O2	C13H16F2N2O2
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexyl-urea
IZ OH	TN OF LINE	TZ O TZ	TZ O TZ	HO N CF3	TX OH
825	928	827	828	829	830

831	HO HO	1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	C14H9F2F3N2O3	Ą	348.22	348.6
832	TZ OT U	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	C14H9F2N3O2	<b>∀</b>	289.24	289.5
833	HY OH	1-Benzo[1,3]dioxol-5-yl-3-(3,5- difluoro-4-hydroxy-phenyl)-urea	C14H10F2N2O4	Ą	308.24	308.5
834	IZ OF	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-o-tolyl-urea	C14H12F2N2O2	∢	278.25	278.6
835	HO N OMe	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	C14H12F2N2O3	Α .	294.25	294.5
836	IZ D IZ U U	1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(2,6-dimethyl-phenyl)-	C15H14F2N2O2	A	292.28	292.6

354.6	314.6	322.7	356.6	264.7
354.31	314.29	322.35	356.32	264.23
A	A	A	А	· V
C16H17F2N2O5	C17H12F2N2O2	C17H20F2N2O2	C19H14F2N2O3	C13H10F2N2O2
1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-diffuoro- 4-hydroxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenyl-urea
HO HO OMB	TZ O TZ	TZ O	IN OH	TZ O TZ
837	838	839	840	841

331.1	301.2	321.0	335.1	335.3
330.76	300.78	320.77	334.80	334.80
A	A	<b>∢</b>	<b>∀</b>	. 4
C14H19CIN2O5	C14H21CIN2O3	C16H17CIN2O3	C17H19CIN2O3	C17H19CIN2O3
3-{3-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-ureido}-propionic acid ethyl ester	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-pentylurea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-pentylurea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-urea	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3- phenethyl-urea
PO P	FO DE STATE OF THE	HN OH	IZ O IZ O OF	HO OF
842	843	844	845	846

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343.7	287.6	327.5	389.4	376.2
342.86	286.75	326.82	388.77	375.63
¥	¥	∢	A	· <b>4</b>
C17H27Cl2N2O2	C13H19CIN2O3	C16HZ3CINZO3	C17H16CIF3N2O3	C15H13Cl3N2O3
1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-[3-chloro-4- hydroxy-5-(1-hydroxy-ethyl)- phenyl]-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-chloro-phenyl)-urea
IZ O	HO TEN TO TEN TEN TO TEN TO TEN TEN TEN TEN TEN TEN TEN TEN TEN TO TEN	IN DO TO	HO HO CP.	D D D D D D D D D D D D D D D D D D D
	848	859	850	851

341.6	375.0	313.0	391.2	332.0
341.19	374.74	312.79	390.74	331.75
V Y	∢	<b>∀</b>	∢	. <b>V</b>
C15H14Cl2N2O3	C16H14CIF3N2O3	C15H21CIN2O3	C16H14CIF3N2O4	C16H14CIN3O3
1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-urea	1-[3-Chforo-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3- cyclohexyl-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethoxy-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-cyano-phenyl)-urea
TZ O TZ	HO HO TO	N O HO OH	HO HO OF STATE OF STA	HO CN
852	823	854	855	856

351.1	321.0	337.1	335.2	397.2
350.75	320.77	336.77	334.80	. 396.82
∢	¥	<b>∀</b>	∢	. <b>V</b>
C16H15CIN205	C16H17CIN2O3	C16H17CIN2O4	C17H19CINZO3	C18H21CIN2O6
1-Benzo[1,3]dioxol-5-yl-3-[3- chloro-4-hydroxy-5-(1-hydroxy- ethyl)-phenyl]-urea	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-o-tolyl- urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(3-methoxy-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2,6-dimethyl-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(3,4,5-trimethoxy-phenyl)-urea
TZ O TZ	TZ OF	HO HO COME	IZ O H	HO H
857	828	859	098	861

862	TZ TZ	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3- naphthalen-1-yl-urea	C19H17CIN2O3	₹	356.80	357.1
863	12 0 12 0 12 0 10 0	1-Adamantan-1-yl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-urea	C19H25CIN2O3	∢	364.87	365.1
864	TZ OF	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(4- phenoxy-phenyl)-urea	C21H19CIN2O4	∢	398.84	399.0
\$98	IN OF OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-phenyl-urea	C15H15CINZO3	∢ .	306.74	307.0
998	HN S HN S	1-(3-Chloro-4-hydroxy-phenyl)-3- pentyl-thiourea	C12H17CINZOS	Н	272.79	272.9

293.1	306.9	307.1	315.0	258.9	245.0
292.78	306.81	306.81	314.87	258.77	244.74
Н	ı	-	п	. ъ	I
C14H13CIN2OS	C15H15CIN2OS	C15H15CIN2OS	C15H23CIN2OS	C11H15CINZOS	C10H13CIN2OS
1-Benzyl-3-(3-chloro-4-hydroxy- phenyl)-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenethyl-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	1-tert-Butyl-3-(3-chloro-4- hydroxy-phenyl)-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea
IZ 00 TO	HN SO	IZ S	TZ OH	IZ S	IN S
867	898	698	870	871	872

873	HN SO THE SOUTH SO	1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	C14H19CIN2OS	Ι	298.83	299.1
874	LE S IN S I	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12CIF3N2OS	I	360.78	361.1
875	D TN TO	1-(3-Chloro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	C13H9C13N2OS	I	347.65	347.9
876	IX IX	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	C13H10Cl2N2OS	I	313.20	313.5
877	IZ S TZ S	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10ClF3N2OS	. 🛏	346.76	347.0
878	IZ S IZ S	1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexyl-thiourea	C13H17CIN2OS	ij	284.80	285.0

347.0	279.0	307.5	327.4	341.4	341.5
346.76	278.76	307.24	327.23	341.26	341.26
I	I			H	
C14H10CIF3N2OS	C13H11CIN2OS	C12H16C12N2OS	C14H12Cl2N2OS	C15H14Cl2N2OS	C15H14Cl2N2OS
1-(3-Chloro-4-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenyl-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-4- hydroxy-phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenethyl-thiourea
HA S T S S S S S S S S S S S S S S S S S	₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩	D F	TIN SO TO	IN SO TO	O H O H
879	088	881	882	883	884

885	D P D	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea	C15H22C12N2OS	I	349.32	349.6
988	ο ο ο ο ο ο ο ο ο ο ο ο ο ο ο ο ο ο ο	1-tert-Butyl-3-(3,5-dichloro-4- hydroxy-phenyl)-thiourea	C11H14Cl2N2OS	I	293.21	293.6
887	D OH	1-(5-Chloro-4-hydroxy-phenyl)-3- isopropyl-thiourea	C10H12Cl2N2OS	ı	279.19	279.5
888	IZ OF	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	C14H18Cl2N2OS	I	333.28	333.5
888	HO IN SOLUTION TO THE SOLUTION	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	C15H11Cl2F3N2OS	<b>p</b> t	395.23	395.5
890	D IN D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-	C13H8CI4N2OS	н	382.09	382.3

			206		
345.9	381.6	319.6	381.4	313.5	283.9
345.65	381.2	319.25	381.20	313.20	283.35
I	l	н	I	П .	
C13H9Cl3N2OS	C14H9Cl2F3N2OS	C13H16Cl2N2OS	C14H9Cl2F3N2OS	C13H10Cl2N2OS	C12H17N3O3S
1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexyl-thiourea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(2-trifluoromethyl-phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- pentyl-thiourea
D TY OH	D P D D		D H HZ S HZ		HN SHOOT OF
891	892	893	894	895	968

897	IN SO I	1-Benzyl-3-(4-hydroxy-3-nitro- phenyl)-thiourea	C14H13N3O3S	I	303.34	304.0
868	IN SO I	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-methyl-benzyl)-thiourea	C15H15N3O3S	Ι	317.36	317.9
868	HN S HO	1-(4-Hydroxy-3-nitro-phenyl)-3- phenethyl-thiourea	CISH15N3O3S	1	317.36	318.0

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
006	HN S H	1-(4-Hydroxy-3-nitro-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23N3O3S	I	325.43	326.1
901	Op.N. N. S. N. O.	1-tert-Butyl-3-(4-hydroxy-3-nitro- phenyl)-thiourea	C11H15N3O3S	I	269.32	239.9
206	N S N S O O O O O O O O O O O O O O O O	1-(4-Hydroxy-3-nitro-phenyl)-3- isopropyl-thiourea	C10H13N3O3S	<b>H</b>	255.29	255.9
903	IN SO I	1-Cyclohexylmethyl-3-(4- hydroxy-3-nitro-phenyl)-thiourea	C14H19N3O3S	н	309.38	309.9
904	N ₂ O _P S	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12F3N3O3S	н	371.33	372.0
905	D D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-thiourea	C13H9Cl2N3O3S	I	358.20	358.6

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906	HN S HN OH	1-(4-Chloro-phenyl)-3-(4-hydroxy-3-nitro-phenyl)-thiourea	C13H10CIN3O3S	Ι	323.75	324.2
206	O ₂ N NH S NH CF ₃	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10F3N3O3S	1	357.31	357.9
806	IN S IN S IN S	1-Cyclohexyl-3-(4-hydroxy-3- nitro-phenyl)-thiourea	C13H17N3O3S	П	295.36	296.0
606	HA SA	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	C14H10F3N3O3S		357.31	357.6
910	IZ SO H	1-(4-Hydroxy-3-nitro-phenyl)-3- phenyl-thiourea	C13H11N3O3S	1	289.31	289.5
911	IN OF	1-(3-Fluoro-4-hydroxy-phenyl)-3- pentyl-thiourea	C12H17FN2OS	I	256.34	256.8
912	IN DE	1-Benzyl-3-(3-fluoro-4-hydroxy- phenyl)-thiourea	C14H13FN2OS	Г	276.33	276.7

913		1-(3-Fluoro-4-hydroxy-phenyl)-3-	CISHISFN2OS	I	290.36	290.5
	HO NO					
914	N N OH	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenethyl-thiourea	C15H15FN2OS	I	290.36	290.5
915	IN SOL	1-(3-Fluoro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23FN2OS	П	298.42	298.7
916	HN S HN S	1-tert-Butyl-3-(3-fluoro-4- hydroxy-phenyl)-thiourea	C11H15FN2OS		242.31	242.8
917	HA NATIONAL STATES	1-(3-Fluoro-4-hydroxy-phenyl)-3- isopropyl-thiourea	C10H13FN2OS	· I	228.29	228.5
918	HN S HN OH	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	C14H19FN2OS	щ	282.38	282.7
916	HO NE SERVICE	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12F4N2OS	Ι	344.33	344.7

920	IZ OT	1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	C13H9Cl2FN2OS	I	331.19	331.5
921	TZ S	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	C13H10CIEN2OS	I	296.75	297.1
922	HO NH CEP3	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10F4N2OS	Ι	330.30	330.6
923	TX OF	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexyl-thiourea	C13H17FN2OS	·	268.35	268.6
924	HZ S HZ S	1-(3-Fluoro-4-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	C14H10F4NZOS	L	330.30	330.5
925	TZ OF	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenyl-thiourea	C13H11FN2OS	1	262.30	262.5
926	EX EX	1-(2,4-Dihydroxy-phenyl)-3- pentyl-thiourea	C12H18N2O2S	ы	254.35	254.6

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274.7	288.6	288.6	296.7	240.6	226.7	280.7
274.34	288.36	288.36	296.43	240.32	226.30	280.39
Ι	Н	П		н	П	<b>-</b>
C14H14N2O2S	C15H16N2O2S	C15H16N2O2S	C15H24N2O2S	C11H16N2O2S	C10H14N2O2S	C14H20N2O2S
1-Benzyl-3-(2,4-dihydroxy- phenyl)-thiourea	1-(2,4-Dihydroxy-phenyl)-3-(2- methyl-benzyl)-thiourea	1-(2,4-Dihydroxy-phenyl)-3- phenethyl-thiourea	1-(2,4-Dihydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	1-tert-Butyl-3-(2,4-dihydroxy- phenyl)-thiourea	1-(2,4-Dihydroxy-phenyl)-3- isopropyl-thiourea	1-Cyclohexylmethyl-3-(2,4-dihydroxy-phenyl)-thiourea
HO OH	FO OH	HO ST	TIN SO TI	TZ S	IZ S	F IN IN
126	928	929	930	931	932	933

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934	HO N N N N N N N N N N N N N N N N N N N	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-benzyl)-thiourea	CISH13F3N2O2S	Н	342.34	342.6
935	D D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-phenyl)-3-(2,4- dihydroxy-phenyl)-thiourea	C13H10CIZNZO2S	Н	329.20	329.5
936	IZ 00 T	1-(4-Chloro-phenyl)-3-(2,4- dihydroxy-phenyl)-thiourea	C13H11CINZO2S		294.76	295.0
937	TZ S S S S S S S S S S S S S S S S S S S	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-phenyl)-thiourea	C14H11F3N2O2S	· H	328.31	328.7
938	FZ S	1-Cyclohexyl-3-(2,4-dihydroxy- phenyl)-thiourea	C13H18N2O2S	н	266.36	266.7
939	H N N N N N N N N N N N N N N N N N N N	1-(2,4-Dihydroxy-phenyl)-3-(2- trifluoromethyl-phenyl)-thiourea	C14H11F3N2O2S	H	328.31	328.6

OH H 1-(2,4-Dihydroxy-phenyl)-3-	1-(2,4-Dihydroxy. phenyl-thiourea	-phenyl)-3-	C13H12N2O2S	П	260.31	260.6
출 오	O IX	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-pentyl-thiourea	C12H16Br2N2OS	I	396.14	396.5
B A		1-Benzyl-3-(3,5-dibromo-4- hydroxy-phenyl)-thiourea	C14H12Br2N2OS	I	416.13	416.4
₩ <b>x</b>	IN OH	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(2-methyl-benzyl)-thiourea	C15H14Br2N2OS	<b>l</b> -sel	430.16	430.5
R OH	TZ on TZ	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenethyl-thiourea	C15H14Br2N2OS	H	430.16	430.5
	IN DE CONTRACTOR OF THE CONTRA	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea	C15HZ2Br2N2OS	Ι	438.22	438.6

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382.4	368.4	422.5	484.5	471.4	437.0
382.11	368.09	422.18	484.13	470.99	436.55
I	l	. 1	Ι	I	<b>-</b>
C11H14B/ZN2OS	C10H12Br2N2OS	C14H18Br2N2OS	C15H11Br2F3N2OS	C13H8Br2CI2N2OS	C13H9Br2CIN2OS
1-tert-Butyl-3-(3,5-dibromo-4- hydroxy-phenyl)-thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-isopropyl-thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(4-chloro-phenyl)-thiourea
HZ S HZ S	HZ S HZ S S S S S S S S S S S S S S S S	IN I	HO HO S	D D D D D D D D D D D D D D D D D D D	IN TO THE TOTAL TO
946	947	948	949	950	951

952	HO NH STATE OF STATE	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	C14H9Br2F3N2OS	Ι	470.10	470.6
953	HOH S	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16Br2N2OS	I	408.15	408.5
954	HO NE STATE OF STATE	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9Br2F3N2OS	H	470.10	470.5
955	TX OH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenyl-thiourea	C13H10Br2N2OS	. 1	402.10	402.6
926	TZ of u	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-pentyl-thiourea	C12H16F2N2OS	H	274.33	274.8
957	IZ U	1-Benzyl-3-(3,5-difluoro-4- hydroxy-phenyl)-thiourea	C14H12F2N2OS	H	294.32	294.7

308.6	308.6	316.8	260.5	246.5	300.6
308.35	308.35	316.41	260.30	246.28	300.37
Н	I		Ι	П	H
C15H14F2N2OS	C15H14F2N2OS	C15H22F2N2OS	C11H14P2N2OS	C10H1ZF2NZOS	C14H18F2N2OS
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-thiourea	1-tert-Butyl-3-(3,5-Difluoro-4- hydroxy-phenyl)-thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-isopropyl-thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea
HOH S		IZ OF U	TZ w	IN SO	TZ TZ OH
958	929	096	961	962	963

964	TN S TO S	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	C15H11FSN2OS	I	362.32	362.8
965	IN OH	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- thiourea	C13H8C12F2N2OS	I	349.18	349.7
996	IX OF U	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	C13H9CIFZN2OS	· I	314.74	315.2
196	HO LINE SERVICES	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	C14H9F5NZOS	I	348.29	348.8
896	TX OF	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16F2N2OS	I	286.34	286.6
696	TX Sy TX	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9F5N2OS	I	348.29	348.8

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970	HZ OH	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenyl-thiourea	C13H10F2N2OS	Ι	280.29	280.5
971	TZ OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-pentyl-thiourea	C14H21CIN2O2S	<b>P</b> ⊷1	316.85	316.9
972	TZ OF	1-Benzyl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-thiourea	C16H17CIN2O2S		336.84	337.2
973	TZ OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-thiourea	C17H19CIN2O2S	H	350.86	351.1
974	TZ OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-phenethyl-thiourea	C17H19CIN2O2S	П	350.86	. 351.0

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359.2	303.0	289.0	343.1	405.2
358.93	302.82	288.79	342.88	404.83
I	I	·	1	<b></b>
C17H27CIN2O2S	C13H19CIN2O2S	C12H17CIN2O2S	C16H23CIN2O2S	CI7H16CIF3N2O2S
1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-thiourea	1-tert-Butyl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-isopropyl-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-thiourea
HO P	HO OH	F OF	E D D D D D D D D D D D D D D D D D D D	HO HO S N N N N N N N N N N N N N N N N N N
975	976	77.6	978	979

086	F D D D D D D D D D D D D D D D D D D D	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(3,5- dichloro-phenyl)-thiourea	C15H13Cl3N2O2S	I	391.70	392.0
981	IN S TO	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-chloro-phenyl)-thiourea	C15H14Cl2N2O2S	I	357.25	357.6
982	HO OF THE STATE OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	I	390.81	391.0
983	HO OF	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexyl-thiourea	C15H21CIN2O2S	I	328.86	329.4
984	HO OH O	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	1	390.81	. 391.0

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323.1	342.2	356.3	376.8	387.2
322.81	341.85	355.88	376.30	386.85
I	D	Д	Q	Q
C15H15CIN2O2S	C19H16CINOS	C20H18CINOS	C19H15Cl2NOS	C19H15CINZO3S
1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-phenyl-thiourea	2-Chloro-4-(2-phenylsulfanyl- benzylamino)-phenol	2-Chloro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Chloro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
IZ S TZ	TZ OF	DE CONTRACTOR OF	5 9 9	HO CC
985	986	987	886	686

oro-4-[2-(4-methoxy- //sulfanyl)-benzylamino]- C20H18CINO2S D 371.88 372.4	loro-4-[2-(2-chloro- ylsulfanyl)-benzylamino]- C19H15Cl2NOS D 376.30 376.8	loro-4-[2-(3-chloro- ylsulfanyl)-benzylamino]- C19H15Cl2NOS D 376.8	loro-4-[2-(3,4-dichloro- ylsulfanyl)-benzylamino]- C19H14Cl3NOS D 410.74 411.2 ol	
C20H18CINO2S	C19H15Cl2NOS	C19H15CIZNOS	C19H14CI3NOS	SCUCNISTIATES
2-Chloro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3-Chloro-4-hydroxy-phenylamino)-methyl]-
HO OHWe	TN D	TN D	TZ OF	IN.
066	991	992	666	

393.4	421.7	401.2	391.9
392.90	421.30	400.88	391.31
D	D	D	Q
C22H17CIN2OS	C19H14Cl2N2O3S	C20H17CIN2O3S	C19H16Cl2N2OS
2-Chloro 4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Chloro-4-(5-nitro-2-p-tolylsuffanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2- chloro-phenol
Z D D D	N N N N N N N N N N N N N N N N N N N	ON THE TOTAL	TZ OF
995	966	266	866

408.7	376.7	390.7	411.1	421.8
408.30	376.30	390.33	410.75	421.30
Q	Q	Q	Q	<b>Q</b>
C19H15CIZN03S	C19H15CIZNOS	C20H17CIZNOS	C19H14CI3NOS	C19H14Cl2N2O3S
2-Chloro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	2,6-Dichloro-4-(2-phenylsulfanyl- benzylamino)-phenol	2,6-Dichloro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	2,6-Dichloro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
	TZ OF	D P	D P D	Phone of the state
666	1000	1001	1002	1003

406.7	411.2	411.2	445.6	433.8
406.33	410.75	410.75	445.19	433.36
D	D	D	Q	Q
C20H17CIZNO2S	C19H14Cl3NOS	C19H14CI3NOS	C19H13Cl4NOS	C21H18CI2N2O2S
2,6-Dichloro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
D H O O O O O O O O O O O O O O O O O O	TZ O O		5 5 5 2 5 2	HO CI
1004	1005	1006	1007	1008

427.8	456.0	435.7	426.0
427.35	455.74	435.33	425.76
D	D	Q	Q
C22H16CI2N2OS	C19H13CI3N2O3S	C20H16Cl2N2O3S	C19H15Cl3N2OS
2,6-Dichloro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,6-Dichloro-4-(5-nitro-2-p- tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2,6-dichloro-phenol
HO CO	HO CO	CG N N N N N N N N N N N N N N N N N N N	Z-LN OH
1009	1010	1011	1012

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443.1	352.8	366.8	387.2	. 397.7
442.75	352.41	366.43	386.85	397.40
Ω	Q	Q	Q	Ω
C19H14Cl3NO3S	C19H16N2O3S	C20H18N2O3S	C19H15CIN2O3S	C19H15N3OSS
2,6-Dichloro-4-[2-(4-chlorobenzenesulfonyl)-benzylamino]-phenol	2-Nitro-4-(2-phenylsulfanyl- benzylamino)-phenol	2-Nitro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	2-Nitro-4-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol
HO CG	O ₂ N N N N N N N N N N N N N N N N N N N	O ₂ N H	HO N ₂ O	SON H NOSO
1013	1014	1015	1016	1017

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382.8	387.2	387.1	421.7	409.9
382.43	386.85	386.85	421.30	409.46
Ω	Q	Q	Q	Q
C20H18N2O4S	C19H15CIN2O3S	C19H15CIN2O3S	C19H14Cl2N2O3S	C21H19N3O4S
4-[2-(4-Methoxy-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- nitro-phenol	N-(4-{2-[(4-Hydroxy-3-nitro-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
O ₂ N	HO NEO OTH	N ₂ O ₂ N H S S CO	HO N _C O	O ₂ N H S S NHAD
1018	1019	1020	1021	1022

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403.8	432.2	411.9	444.3
403.45	431.85	411.43	443.90
Ð	Q	Q	Q
C22H17N3O3S	C19H14CIN3O5S	C20H17N3O5S	C21H18CIN3O4S
2-Nitro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-nitro-phenol	2-Nitro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	N-{4-(4-Chloro-phenylsulfanyl)-3- [(4-hydroxy-3-nitro-phenylamino)- methyl]-phenyl}-acetamide
O ₂ N H	O ₂ N H NO ₂	O ₂ N K	O ₂ N H S S H C C C C C C C C C C C C C C C C
1023	1024	1025	1026

419.2	324.6	340.8	360.1	370.8
418.85	325.40	339.43	359.84	370.40
D	Q	Q	Q	Q
C19H15CIN2O5S	C19H16FNOS	C20H18FNOS	C19H15CIFNOS	C19H15FN2O3S
4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-nitro-phenol	2-Fluoro-4-(2-phenylsulfanyl- benzylamino)-phenol	2-Fluoro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Fluoro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol
H Noo			TZ,	HN ON
1027	1028	1029	1030	1031

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355.8	360.2	360.3	394.6	382.9
355.43	359.84	359.84	394.29	382.45
А	Q		Q	Ω
C20H18FNO2S	C19H15CIFNOS	C19H15CIFNOS	C19H14Cl2FNOS	C21H19FN2O2S
2-Fluoro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(3-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-4-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Fluoro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S COME	HO N N N N N N N N N N N N N N N N N N N	HO S CO	HO N	HO S S NHAC
1032	1033	1034	1035	1036

377.0	405.3	384.9	375.1
376.45	404.84	384.42	374.86
Q	Q	Q	Q
C22H17FN2OS	C19H14CIFN2O3S	C20H17FN2O3S	C19H16CIFN2OS
2-Fluoro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Fluoro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2- fluoro-phenol
HO NO	HO S CI	HON HON OH	ZZ-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-SS-LY-
1037	1038	1039	1040

392.0	323.8	337.8	358.2	368.7
391.84	323.41	337.44	357.85	368.41
Q	Q	Q	Q	Ð
C19H15CIFNO3S	C19H17NO2S	C20H19NO2S	C19H16CINO2S	C19H16N2O4S
2-Fluoro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	4-(2-Phenylsulfanyl-benzylamino)- benzene-1,3-diol	4-(2-p-Tolylsulfanyl- benzylamino)-benzene-1,3-diol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(4-Nitro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol
P P P P P P P P P P P P P P P P P P P	HO NET	HO NH	TZ D	HO S NO2
1041	1042	1043	1044	1045

				1
353.7	358.3	358.1	392.7	380.8
353.43	357.85	357.86	392.30	380.46
Q	Q	Q	Q	Q
C20H19NO3S	C19H16CINO2S	C19H16CINO2S	C19H15Cl2NO2S	C21H20N2O3S
4-[2-(4-Methoxy-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]- benzene-1,3-diol	N-(4-{2-[(2,4-Dihydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl}-acetamide
HO N N N N N N N N N N N N N N N N N N N	HO HO N	HO CG	HO OH OH	HO NHAC
1046	1047	1048	1049	1050

374.9	403.2	382.7	373.0
374.46	402.85	382.43	372.87
D	D	Q	Q
C22H18N2O2S	C19H15CIN2O4S	C20H18NZO4S	C19H17CIN2O2S
4-[2-(Quinolin-7-ylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-benzene-1,3- diol	4-(5-Nitro-2-p-tolylsulfanyl- benzylamino)-benzene-1,3-diol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-benzene-1,3-diol
TZ TO TO TEST	P S S S S S S S S S S S S S S S S S S S	P S S S S S S S S S S S S S S S S S S S	HZ SO
1051	1052	1053	1054

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1055	4-0-0-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-	4-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-benzene-1,3-diol	C19H16CINO4S	Д	389.85	390.2
1056	S H OH	2,6-Dibromo-4-(2-phenylsulfanylbenzylamino)-phenol	C19H15Br2NOS	Q	465.20	465.7
1057	PA SE	2,6-Dibromo-4-(2-p-tolylsulfanyl- benzylamino)-phenol	C20H17Br2NOS	Q	479.23	479.3
1058	HN Page 1	2,6-Dibromo-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	C19H14Br2CINOS	D	499.65	500.1
1059	HO Br	2,6-Dibromo-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	C19H14Br2N2O3S	Q	510.2	510.1

495.3	499.8	499.8	534.2	522.4
495.23	499.65	499.65	534.09	522.25
Q	D	О	Q	Q
C20H17Br2NO2S	C19H14Br2CINOS	C19H14Br2CINOS	C19H13Br2Cl2NOS	C21H18Br2N2O2S
2,6-Dibromo-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dibromo-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S S S S S S S S S S S S S S S S S S S	TZ OT	DH NO THE STATE OF	D D D D D D D D D D D D D D D D D D D	HO HO S
1360	1061	1062	1063	1064

516.4	544.8	524.6	514.9
516.25	544.64	524.23	514.66
Q	Ω	Q	٦
C22H16Br2N2OS	C19H13Br2CIN2O3 S	C20H16Br2N2O3S	C19H15Br2CIN2OS
2,6-Dibromo-4-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,6-Dibromo-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2,6-dibromo-phenol
TZ S	DH D	N N N N N N N N N N N N N N N N N N N	HO BIT OF THE STATE OF THE STAT
1065	1066	1067	1068

531.7	343.6	357.8	378.1	388.8
531.65	343.39	357.42	377.83	388.39
Q	О	. Δ	Q	Д
C19H14Br2CINO3S	C19H15F2NOS	C20H17F2NOS	C19H14CIF2NOS	C19H14F2N2O3S
2,6-Dibromo-4-[2-(4-chlorobenzenesulfonyl)-benzylaminol-phenol	2,6-Difluoro-4-(2-phenylsulfanyl- benzylamino)-phenol	2,6-Difluoro 4-(2-p-tolylsulfanyl- benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2,6-difluoro-phenol	2,6-Difluoro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
HO O2S	TZ Q	TZ U	TZ OF	HN S S NO2
1069	1070	1071	1072	1073

T	-	Т		
373.7	378.1	378.2	412.6	400.8
373.42	377.83	377.83	412.28	400.44
Q	D	D	Ω	Q
C20H17F2NO2S	C19H14CIF2NOS	C19H14CIF2NOS	C19H13Cl2F2NOS	C21H18F2N2O2S
2,6-Difluoro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2,6-difluoro-phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2,6-difluoro-phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2,6- difluoro-phenol	N-(4-{2-[(3,5-Difluoro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S S S S S S S S S S S S S S S S S S S	HZ OD	TZ w	TZ OH	HO S S S S S S S S S S S S S S S S S S S
1074	1075	1076	1077	1078

394.9	423.3	402.8	393.0
394.44	422.83	402.41	392.85
D	Q	Q	Q
C22H16F2N2OS	C19H13CIF2N2O3S	C20H16F2N2O3S	C19H15CIFZN2OS
2,6-Difluoro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2,6-difluoro- phenol	2,6-Difluoro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2,6- difluoro-phenol
I.X.	IZ U	TZ S	HN HOH
1079	1080	1081	1082

392.3	342.3	400.2	420.9	431.3
391.84	341.85	399.93	420.35	430.90
Q	D	O.	Q	Q
C19H14CIF2NO3S	C21H20CINO2S	C22H22CINO2S	C21H19Cl2NO2S	C21H19CIN2O4S
4-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-2,6-difluoro-phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- (2-phenylsulfanyl-benzylamino)- phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- (2-p-tolylsulfanyl-benzylamino)- phenol	2-Chloro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(4-nitro-phenylsulfanyl)- benzylamino]-phenol
HN PO	\$_\frac{1}{5}	TZ TZ	F OF	FY OH ON
1083	1084	1085	1086	1087

416.3	420.9	420.8	455.2	443.4
415.93	420.35	420.35	454.80	442.96
Q	О		۵	Q
C22H22CINO3S	C21H19Cl2NO2S	C21H19Cl2NO2S	C21H18Cl3NO2S	C23H23CIN2O3S
2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(4-methoxy-phenylsulfanyl)- benzylamino]-phenol	2-Chloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Chloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Chloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	N-[4-(2-{[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl}-phenylamino]-methyl}-phenylsulfanyl}-phenyl]-acetamide
HO NOW S	F OF	HO P	5 5 5 5	HO HO INHAD
1088	1089	1090	1001	1092

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1093	HO H	2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(quinolin-7-ylsulfanyl)- benzylamino]-phenol	C24H21CIN2O2S	Q	436.95	437.3
1094	P P P	2-Chloro-4-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H18CI2N2O4S	D	465.35	465.9
1095		2-Chloro-4-(1-hydroxy-ethyl)-6- (5-nitro-2-p-tolylsulfanyl- benzylamino)-phenol	C22H21CIN2O4S	Q	444.93	445.3
1096	FZ OF DE CONTRACTOR OF THE CON	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-chloro-6-(1-hydroxy-ethyl)-phenol	C21H20Cl2N2O2S	Д	435.37	435.6

452.5	337.8	351.8	371.9	382.7
452.35	337.44	351.46	371.88	382.43
Q	D	D	Q	Q
C21H19CI2NO4S	C20H19NO2S	C21H21NO2S	C20H18CINO2S	C20H18N2O4S
2-Chloro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Hydroxymethyl-4-(2- phenylsulfanyl-benzylamino)- phenol	2-Hydroxymethyl-4-(2-p-tolylsulfanyl-benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxymethyl- phenol	2-Hydroxymethyl-4-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol
HO HO TO	F S S	F - S	₽ 9 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	HO SHOOM
1097	1098	1099	1100	1101

367.46 367.9	371.88 371.9	 371.88 371.9	
D 3	D 3	 Q	O O
C21H21N03S	C20H18CINO2S	C20H18CINO2S	C20H18CINO2S
2-Hydroxymethyl-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxymethyl- phenol	4-[2-(3-Chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol	4-[2-(3-Chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol 4-[2-(3,4-Dichloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol
F P	\$	TN. TN.	5 5 5 
1102	1103	1104	1104

388.8	417.2	396.8	387.1
388.48	416.88	396.46	386.90
D	D	Q	Q
C23H20N2O2S	C20H17CIN2O4S	C21H20N2O4S	C20H19CIN2O2S
2-Hydroxymethyl-4-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2- hydroxymethyl-phenol	2-Hydroxymethyl-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol
E OH	S IN S	ON THE STATE OF	F S S S S S S S S S S S S S S S S S S S
1107	1108	1109	1110

	FZ FZ	4-[2-(4-Chloro-benzenesulfonyl)-	C. C	٢	403.88	0 74	
百		benzylaminoj-2-hydroxymetnyi- phenol	CZUHIBCINO45	a	100.00		
. \ 1		1-[3-Chloro-2-hydroxy-5-(2-phenylsulfanyl-benzylamino)-phenyl]-ethanone	C21H18CINO2S	Д	383.89	384.2	
1 0 =	TZ TO	1-[3-Chloro-2-hydroxy-5-(2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone	C22H20CINO2S	D	397.92	398.2	
) o—\ ¥		1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	C21H17Cl2NO2S	Q	418.34	418.8	
∫ o≕ Ş	TZ 5	1-{3-Chloro-2-hydroxy-5-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenyl}-ethanone	C21H17CIN2O4S	Q	428.89	429.3	

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414.5	418.6	418.5	453.0	441.2
413.92	418.34	418.34	452.78	440.94
D	D	D	Q	Q
C22H20CINO3S	C21H17G2NO2S	C21H17G2NO2S	C21H16CI3NO2S	C23H21CIN2O3S
1-{3-Chloro-2-hydroxy-5-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenyl}-ethanone	1-[3-Chloro-5-[2-(2-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{3-Chloro-5-{2-(3-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{3-Chloro-5-{2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	N-(4-{2-[(3-Acetyl-5-chloro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
TA CO	TX O O T	D TX O Q TX	5 5 5 5 9 9	HO CI S NHAC
1116	1117	1118	1119	1120

435.2	463.7	443.2	433.6
434.94	463.33	442.92	433.35
D	Q	. Д	Q
C24H19CIN2O2S	C21H16Cl2N2O4S	C22H19CIN2O4S	C21H18Cl2N2O2S
1-{3-Chloro-2-hydroxy-5-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenyl}-ethanone	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-2-hydroxy-phenyl}-ethanone	1-[3-Chloro-2-hydroxy-5-(5-nitro- 2-p-tolylsulfanyl-benzylamino)- phenyl]-ethanone	1-{5-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-3-chloro-2-hydroxy-phenyl}-ethanone
		JN JO DE TO	D D D D D D D D D D D D D D
1121	1122	1123	1124

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1125	D S S S S S S S S S S S S S S S S S S S	1-{3-Chloro-5-[2-(4-chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	C21H17Cl2NO4S	Q	450.33	450.5
1126	HOOCC H	2-Hydroxy-5-(2-phenylsulfanyl- benzylamino)-benżoic acid	C20H17NO3S	Q	351.42	351.6
1127	HOOC N	2-Hydroxy-5-(2-p-tolylsulfanyl- benzylamino)-benzoic acid	C21H19NO3S	Д	365.44	365.8
1128	HOOCC NO.	5-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	C20H16CINO3S	Ω	385.86	385.1
1129	HOOC S	2-Hydroxy-5-[2-(4-nitro- phenylsulfanyl)-benzylamino]- benzoic acid	C20H16N2O5S	Q	396.11	396.4

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381.6	386.0	386.0	420.7	408.7
381.44	385.86	385.86	420.31	408.47
Д	D	D	Ω	Д
C21H19NO4S	C20H16CINO3S	C20H16CINO3S	C20H15Cl2NO3S	C22H20N2O4S
2-Hydroxy-5-[2-(4-methoxy-phenylsulfanyl)-benzylamino}-benzoic acid	5-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	5-[2-(3-Chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-benzoic acid	5-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- hydroxy-benzoic acid	5-[2-(4-Acetylamino-phenylsulfanyl)-benzylamino]-2-hydroxy-benzoic acid
HOOC	HOOOC PA	HOOC	HOOC N	HOOC
1130	1131	1132	1133	1134

402.8	430.9	410.7	387.2
402.46	430.86	410.44	386.90
D	D	<b>Q</b>	Д
C23H18N2O3S	C20H15CIN2O5S	C21H18N2O5S	C20H19CINZO2S
2-Hydroxy-5-[2-(quinolin-7- ylsulfanyl)-benzylamino]-benzoic acid	5-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-hydroxy- benzoic acid	2-Hydroxy-5-(5-nitro-2-p-tolylsulfanyl-benzylamino)-benzoic acid	5-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol
NOOCH NOOCH	N N OOH	HOOC NO S	HOOC S S DH
1135	1136	1137	1138

404.1	370.8	384.9	405.0	415.8
403.88	370.40	384.43	404.84	415.40
Q	D	Q	Ω	Q
C20H16CINO5S	C19H15FN2O3S	C20H17FNZO3S	C19H14ClFN2O3S	C19H14FN3O5S
5-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-benzoic acid	2-Fluoro-6-nitro-4-(2- phenylsulfanyl-benzylamino)- phenol	2-Fluoro-6-nitro-4-(2-p-tolylsulfanyl-benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-fluoro-6-nitro- phenol	2-Fluoro-6-nitro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
HOOC N OP S	TX OY	EN SON SON SON SON SON SON SON SON SON SO	HZ ON	HO ₂ O _N O ₂
1139	1140	1141	1142	1143

400.9	405.0	405.0	439.9	427.9
400.43	404.84	404.84	439.29	427.45
D	Q	Q	Q	
C20H17FN2O4S	C19H14CIFN2O3S	C19H14CIFN2O3S	C19H13Cl2FN2O3S	C21H18FN3O4S
2-Fluoro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-6-nitro-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-fluoro-6-nitro- phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-fluoro-6-nitro- phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- fluoro-6-nitro-phenol	N-(4-{2-[(3-Fluoro-4-hydroxy-5-nitro-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO NO2	HA SON	HON NOS	TZ ZON DH	HO S S NHAC
1144	1145	1146	1147	1148

421.6	450.1	429.8	420.2
421.45	449.84	429.42	419.86
Q	О	. Д	
C22H16FN3O3S	C19H13CIFN3O5S	C20H16FN3O4S	C19H15CIFN3O2S
2-Fluoro-6-nitro-4-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-fluoro-6- nitro-phenol	2-Fluoro-6-nitro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-fluoro-6-nitro-phenol
TIN ON ON	SZ S	HO NO S	HO S S S S S S S S S S S S S S S S S S S
1149	1150	1151	1152

437.1	360.5	395.0	416.8
436.84	360.23	394.68	416.34
Д	Q		Ω
C19H15CIFN2O5S	C19H15Cl2NO2	C19H15Cl3NO2	C23H23Cl2NO2
4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-fluoro-6-nitro-phenol	2,6-Dichloro-4-(3-phenoxy-benzylamino)-phenol	2,6-Dichloro-4-[3-(4-chloro-phenoty)-benzylamino]-phenot	4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2,6-dichloro-phenol
HO NO ON	TZ TO	D D D D D D D D D D D D D D D D D D D	2 <u>1</u> 2 <u>5</u>
1153	1154	1155	1156

374.6	374.6	318.6	314.7	328.6
374.26	374.26	318.20	314.23	328.26
О	D	D	Q	Q
C20H17Cl2NO2	C20H17CI2NO2	CI7H13Cl2NO	C14H13Cl2NOS	C15H15Cl2NOS
4-(3-Benzyloxy-benzylamino)-2,6-dichloro-phenol	4-(2-Benzyloxy-benzylamino)-2,6-dichloro-phenol	2,6-Dichloro-4-[(naphthalen-1-ylmethyl)-amino]-phenol	2,6-Dichloro-4-(4-methylsulfanyl- benzylamino)-phenol	2,6-Dichloro-4-(2-ethylsulfanyl-benzylamino)-phenol
D OH	TZ O	TZ 5 9	S O P	S TZ TO
1157	1158	1159	1160	1161

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353.6	416.9	334.6	353.4	390.6
353.24	416.77	334.20	353.06	390.26
Q	D	. О	Q	. <b>Q</b>
C17H18Cl2N2O2	C17H12C13NOS2	C16H13CI2N3O	C11H8BrCl2NOS	C20H17Cl2NO3
2,6-Dichloro-4-(2-morpholin-4-yl-benzylamino)-phenol	2,6-Dichloro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2,6-Dichloro-4-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2,6-dichloro- phenol	2,6-Dichloro-4-[3-(4-methoxy-phenoxy)-benzylamino]-phenol
7 - z - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5	HO CO	TV D D D	IN D	
1162	1163	1164	1165	1166

282.4	336.5	320.8	307.8	342.1
282.17	336.14	320.57	307.34	341.79
Q	D	Q	Q	Q
C14H13CIZNO	C14H10Cl2F3NO	C13H9Cl3FNO	C19H17NO3	C19H16CINO3
2,6-Dichloro-4-(3-methyl- benzylamino)-phenol	2,6-Dichloro-4-(3-trifluoromethyl-benzylamino)-phenol	2,6-Dichloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	4-(3-Phenoxy-benzylamino)- benzene-1,3-diol	4-[3-(4-Chloro-phenoxy)- benzylamino]-benzene-1,3-diol
TZ OF	D P	-5 -5 -5 -7 -7	5—————————————————————————————————————	5—————————————————————————————————————
1167	1168	1169	1170	1171

1

		T		
363.9	321.6	321.5	265.7	261.7
363.45	321.37	321.37	265.31	261.34
. д	Д	Q	D	Q
C23H25NO3	C20H19NO3	C20H19NO3	C17H15N02	C14H15NO2S
4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-benzene-1,3-diol	4-(3-Benzyloxy-benzylamino)- benzene-1,3-diol	4-(2-Benzyloxy-benzylamino)- benzene-1,3-diol	4-[(Naphthalen-1-ylmethyl)- amino]-benzene-1,3-diol	4-(4-Methylsulfanyl- benzylamino)-benzene-1,3-diol
# P	F Q	12 5—0 9	F. D.	S IN
1172	1173	1174	1175	1176

275.9	300.8	364.1	281.6	367.4
275.37	300.35	363.88	281.31	367.09
Q	Д	D	D	Q
C15H17NO2S	C17H20N2O3	C17H14CINO2S2	C16H15N3O2	C12H10BrC12NOS
4-(2-Ethylsulfanyl-benzylamino)- benzene-1,3-diol	4-(2-Morpholin-4-yl- benzylamino)-benzene-1,3-diol	4-{[2-(4-Chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-benzene-1,3-diol	4-[(5-Phenyl-2H-imidazol-4- ylmethyl)-amino]-benzene-1,3-diol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro-3- methyl-phenol
F. S.	TN TO	S S S S S S S S S S S S S S S S S S S	N HO OH	E 5
1177	1178	1179	1180	1181

337.8	229.6	283.6	268.0	326.1
337.37	229.27	283.25	267.68	325.79
Q	D	D	Q	Q
C20H19NO4	C14H15NO2	C14H12F3NO2	C13H11CIFNO2	C19H16CINO2
4-[3-(4-Methoxy-phenoxy)- benzylamino]-benzene-1,3-diol	4-(3-Methyl-benzylamino)- benzene-1,3-diol	4-(3-Trifluoromethyl- benzylamino)-benzene-1,3-diol	4-(2-Chloro-6-fluoro- benzylamino)-benzene-1,3-diol	2-Chioro-4-(3-phenoxy-benzylamino)-phenol
4	15 Tz	H H OH	5 12 5	HN DH
1182	1183	1184	1185	1186

360.6	382.2	340.1	340.1
360.23	381.90	339.82	339.82
Q	Д	D	Q
C19H15GI2NO2	C23H24CINO2	C20H18CINO2	C20H18CINO2
2-Chloro-4-[3-(4-chloro-phenoxy)-benzylamino]-phenol	4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2-chloro-phenol	4-(3-Benzyloxy-benzylamino)-2- chloro-phenol	4-(2-Benzyloxy-benzylamino)-2- chloro-phenol
D TY			TZ OF
1187	1188	1189	1190

			T	
284.0	280.2	294.3	319.1	382.6
283.75	279.79	293.81	318.80	382.33
D	D	D	Q	Q
C17H14CINO	C14H14CINOS	C15H16CINOS	C17H19CiN2O2	C17H13Cl2NOS2
2-Chloro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Chloro-4-(4-methylsulfanyl- benzylamino)-phenol	2-Chloro-4-(2-ethylsulfanyl- benzylamino)-phenol	2-Chloro-4-(2-morpholin-4-yl-benzylamino)-phenol	2-Chloro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol
IN S	TZ.	D TZ		S S S S S S S S S S S S S S S S S S S
1191	1192	1193	1194	1195

1196	N CI VII VII VII VII VII VII VII VII VII	2-Chloro-4-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol	C16H14CIN3O	Q	299.75	300.2
1197	TIN OF	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2-chloro-phenol	C11H9BrCINOS	D	318.62	319.5
1198		2-Chloro-4-[3-(4-methoxy-phenol-phenol	C20H18CINO3	. О	355.81	356.5
1199		2-Chloro-4-(3-methyl-benzylamino)-phenol	C14H14CINO	Q	247.72	248.5

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
1200	CI CF3	2-Chloro-4-(3-trifluoromethyl- benzylamino)-phenol	C14H11CIF3NO	D	301.69	302.2
1201	D P	2-Chloro-4-(2-chloro-6-fluoro- benzylamino)-phenol	C13H10Cl2FNO	D	286.13	286.6
1202	TIZ OF	2-Fluoro-4-(3-phenoxy- benzylamino)-phenol	C19H16FNO2	Q	309.33	309.8
1203	TZ OT	2-Fluoro-4-[3-(4-chloro-phenoxy)- benzylamino]-phenol	C19H15CIFNO2	Q	343.77	344.0

366.0	323.8	323.8	267.7	263.5
365.44	323.36	323.36	267.30	263.33
D	Q	. Д	Q	Q
C23H24FNO2	C20H18FNO2	C20H18FNO2	C17H14FNO	C14H14FNOS
4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2-fluoro-phenol	4-(3-Benzyloxy-benzylamino)-2- fluoro-phenol	4-(2-Benzyloxy-benzylamino)-2- fluoro-phenol	2-Fluoro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Fluoro-4-(4-methylsulfanyl- benzylamino)-phenol
TZ P			The state of the s	LIN OH
1204	1205	1206	1207	1208

277.8	302.8	366.0	283.8	302.5
277.36	302.34	365.87	283.30	302.16
D	D	Q	Q	Q
C15H16FNOS	C17H19FN2O2	C17H13CIFNOS2	C16H14FN3O	C11H9BrFNOS
2-Fluoro-4-(2-ethylsulfanyl- benzylamino)-phenol	2-Fluoro-4-(2-morpholin-4-yl- benzylamino)-phenol	2-Fluoro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2-Fluoro-4-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2-fluoro-phenol
TZ OT	TZ.	TI OF	TZ OH	IN OH
1209	1210	1211	1212	1213

339.8	231.4	285.5	270.1	327.6
339.36	231.27	285.24	269.67	327.32
Q	Q	О .	Q	Q
C20H18FNO3	C14H14FNO	C14H11F4NO	C13H10CIF2NO	C19H15F2NO2
2-Fluoro-4-[3-(4-methoxy-phenoxy)-benzylamino]-phenol	2-Fluoro-4-(3-methyl- benzyłamino)-phenol	2-Fluoro-4-(3-trifluoromethyl- benzylamino)-phenol	2-Fluoro-4-(2-chloro-6-fluoro- benzylamino)-phenol	2,6-Difluoro-4-(3-phenoxy- benzylamino)-phenol
TZ Q	TZ OF	HN OH	TZ OF	TZ Y
1214	1215	. 1216	1217	1218

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362.0	383.8	341.7	341.7
361.76	383.43	341.35	341.35
Q	Q	Д	Q
C19H14CIFZNO2	C23H23F2NO2	C20H17F2NO2	C20H17F2NO2
2,6-Difluoro-4-[3-(4-chloro- phenoxy)-benzylamino]-phenol	4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2,6-difluoro-phenol	4-(3-Benzyloxy-benzylamino)-2,6-difluoro-phenol	4-(2-Benzyloxy-benzylamino)-2,6- difluoro-phenol
IZ LZ LZ	TZ u	IZ u	IZ U
1219	1220	1221	1222

285.6	281.6	295.7	320.8	384.2
285.29	281.32	295.35	320.33	383.86
D	D	О	Q	Q
C17H13F2NO	C14H13FZNOS	C15H15F2NOS	C17H18F2N2O2	C17H12CIF2NOS2
2,6-Difluoro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2,6-Difluoro-4-(4-methylsulfanyl- benzylamino)-phenol	2,6-Difluoro-4-(2-ethylsulfanyl- benzylamino)-phenol	2,6-Difluoro-4-(2-morpholin-4-yl- benzylamino)-phenol	2,6-Difluoro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol
IZ Q	TN H	TZ U	TZ U	TZ OH
1223	1224	1225	1226	1227

301.6	320.4	357.6	249.6	303.7
301.29	320.15	357.35	249.26	303.23
D	D	. Q	Q ·	Q
C16H13F2N3O	C11H8BrFZNOS	C20H17F2NO3	C14H13FZNO	C14H10F5NO
2,6-Difluoro-4-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2,6-difluoro- phenol	2,6-Difluoro-4-[3-(4-methoxy- phenoxy)-benzylamino]-phenol	2,6-Difluoro-4-(3-methyl- benzylamino)-phenol	2,6-Difluoro-4-(3-trifluoromethyl- benzylamino)-phenol
Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z	TA OH		TZ UL OF	HO LE
1228	1229	1230	1231	1232

1233	TZ OH	2,6-Difluoro-4-(2-chloro-6-fluoro- benzylamino)-phenol	C13H9CIF3NO	Q	287.66	288.1
1234	HN HO HO	N-(2,4-Dihydroxy-phenyl)-C- phenyl-methanesulfonamide	C13H13NO4S	Ф	279.31	279.8
1235	HNOHO	Butane-1-sulfonic acid (2,4-dihydroxy-phenyl)-amide	C10H15NO4S	Д	245.30	245.6
1236	O S O HO	Octane-1-sulfonic acid (2,4-dihydroxy-phenyl)-amide	C14H23NO4S		301.40	301.8
1237	O HN OHO	Propane-2-sulfonic acid (2,4-dihydroxy-phenyl)-amide	C9H13NO4S	æ	231.27	231.7

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332.4	298.5	354.6	284.5	297.9
332.20	298.19	354.29	284.16	297.76
A .	В	В	В	В
C13H11Cl2NO3S	C10H13CIZNO3S	C14H21Cl2NO3S	C9H11Cl2NO3S	C13H12CINO3S
N-(3,5-Dichloro-4-hydroxy- phenyl)-C-phenyl- methanesulfonamide	Butane-1-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	N-(3-Chloro-4-hydroxy-phenyl)- C-phenyl-methanesulfonamide
HO NH O	HA CO	O D O T	HONNIN	HO—NH O
1238	1239	1240	1241	1242

1243	HO NH O	Butane-1-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C10H14CINO3S	В	263.74	264.0
1244	TZ O	Octane-1-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C14H22GINO3S	Δ.	319.85	320.3
1245	HO	Propane-2-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C9H12CINO3S	Д	249.71	250.4
1246	HO NH O	N-(3-Fluoro-4-hydroxy-phenyl)-C-phenyl-methanesulfonamide	C13H12FNO3S	В	281.30	281.8
1247	HOWA	Butane-1-sulfonic acid (3-fluoro-4-hydroxy-phenyl)-amide	C10H14FNO3S	В	247.29	247.8

303.8	233.7	300.8	265.7	321.8
303.39	233.26	299.29	265.28	321.38
В	В	Д	<b>A</b>	æ
C14H22FNO3S	C9H12FNO3S	C13H11F2NO3S	C10Hi3F2NO3S	C14H21F2NO3S
Octane-1-sulfonic acid (3-fluoro-4- hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3-fluoro-4-hydroxy-phenyl)-amide	N-(3,5-Difluoro-4-hydroxy- phenyl)-C-phenyl- methanesulfonamide	Butane-1-sulfonic acid (3,5-difluoro-4-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,5- difluoro-4-hydroxy-phenyl)-amide
IN DE	HO	HOH	HOH	O S O T
1248	1249	1250	1251	1252

251.6	253.7	306.4	272.1	255.6
251.25	253.29	306.18	271.74	255.29
В	F, G, H	F, G, H	F, G, H	F, G, H
C9H11F2NO3S	C13H19NO4	C13H17CI2NO3	C13H18CINO3	C13H18FNO3
Propane-2-sulfonic acid (3,5-difluoro-4-hydroxy-phenyl)-amide	(2,4-Dihydroxy-phenyl)-carbamic acid hexyl ester	(3,5-Dichloro-4-hydroxy-phenyl)- carbamic acid hexyl ester	(3-Chloro-4-hydroxy-phenyl)- carbamic acid hexyl ester	(3-Fluoro-4-hydroxy-phenyl)- carbamic acid hexyl ester
HN OH	₽ 0± 0± 0± 0± 0± 0± 0± 0± 0± 0± 0± 0± 0±	P	Fo o	F
1253	1254	1255	1256	1257

		280		
395.3	273.6	310.7	363.6	329.1
395.09	273.28	310.35	363.24	328.79
F, G, H	F, G, H		¥	А
C13H17Br2NO3	C13H17F2NO3	acid C15H22N2O5	C15H20Cl2N2O4	C15H21CIN2O4
(3,5-Dibromo-4-hydroxy-phenyl)- carbamic acid hexyl ester	(3,5-Difluoro-4-hydroxy-phenyl)- carbamic acid hexyl ester	-[3-(2,4-Dihydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3,5-Dichloro-4-hydroxy-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester
10 To	HNN O	TZ OH	TZ O	IZ O IZ
1258	1259	1260	1261	1262

312.8	330.8	452.3	344.8	397.6
312.34	330.33	452.14	344.36	397.25
А	Ą	Ą	Ą	Ą
C15H21FN2O4	C15H20F2N2O4	C15H20Br2N2O4	C18HZ0NZOS	C18H18Cl2N2O4
2-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3,5-Difluoro-4-hydroxy-4-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3,5-Dibromo-4-hydroxy-4-methyl-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(2,4-Dihydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3,5-Dichloro-4-hydroxy-phenyl)-ureido]-3-phenyl-propionic acid ethyl ester
TZ O TZ	TZ O L	HZ O H	IZ O	TZ O
1263	1264	1265	1266	1267

363.0	346.7	364.8	486.2
362.81	346.35	364.34	486.15
¥	<b>∀</b>	A	A
C18H19CINZO4	C18H19FN2O4	C18H18F2N2O4	C18H18Br2N2O4
2-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyi ester	2-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3,5-Difluoro-4-hydroxy-phenyl)-ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3,5-Dibromo-3-fluoro-4- hydroxy-phenyl)-ureido]-3-phenyl- propionic acid ethyl ester
TZ O	HZ HZ OF		HN O HO H
1268	1269	1270	1271

1272	HO OH	3,5,5-Trimethyl-hexanoic acid (2,4-dihydroxy-phenyl)-amide	C15HZ3NO3	υ	265.35	265.7
1273	HO CO	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-4-hydroxy-phenyl)- amide	C15H21Cl2NO2	υ	318.24	318.5
1274	HO NO	3,5,5-Trimethyl-hexanoic acid (3- chloro-4-hydroxy-phenyl)-amide	C15H22CINO2	၁	283.79	284.0
1275	HO NO	3,5,5-Trimethyl-hexanoic acid (3-fluoro-4-hydroxy-phenyl)-amide	C15H21FNO2	၁	267.34	267.7
1276	D TZ	3,5,5-Trimethyl-hexanoic acid (3,5-difluoro-4-hydroxy-phenyl)- amide	C15H21F2NO2	S	285.33	285.7

407.3	376.1	410.1	424.1
407.14	375.9	409.9	423.9
၁	K. followed by A	K followed by A	K followed by A
C15H21Br2NO2	C18H18CIN3O2S	C21H16CIN3O2S	C22H18CIN3O2S
3,5,5-Trimethyl-hexanoic acid (3,5-dibromo-4-hydroxy-phenyl)-amide	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-tert-butyl-urea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-benzyl-urea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-phenethyl-urea
IN PER SECOND	S IN O	D IZ S	PO NH NH O
1277	1278	1279	1280

378.1	392.1	417.2
377.9	391.9	417.0
K followed by I	K followed by I	K followed by C
C17H16CIN3OS2	C18H18CIN3OS2	C22H25CIN2O2S
1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-isopropyl- thiourea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-tert-butyl- thiourea	3,5,5-Trimethyl-hexanoic acid (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-amide
D IN NEW YORK	D EN NEW YORK OF THE SECOND SE	TO NEW YORK TO NEW
1281	1282	1283

1284	N N N N N N N N N N N N N N N N N N N	N-(3-Benzothiazol-2-yl-5-chloro- 4-hydroxy-phenyl)-3-phenyl- propionamide	C22H17GIN2O2S	K followed by C	408.9	409.2
1285	IZ OH	1-(4-Hydroxy-2-methyl-phenyl)-3- pentyl-urea	C13H20N2O2	A	263.31	256.9
1286	PO NATIONAL PROPERTY OF THE PR	Biphenyl-4-carboxylic acid (2,4- dihydroxy-phenyl)-amide	C19H15NO3	C, B	305.33	305.6
1287	TZ OF	Biphenyl-4-carboxylic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	C20H15Cl2NO2	C, E	358.22	358.5
1288	HO OH	4-[(Furan-2-ylmethyl)-amino]- benzene-1,3-diol	C11H11NO3	D	205.21	205.7

258.4	225.7	283.5	303.6	310.4
258.10	225.19	283.25	303.23	310.18
D	D	D	D	E, E
C11H9Cl2NO2	C11H9F2NO2	C14H12F3NO2	C14H10F5NO	C15H13Cl2NO2
2,6-Dichloro-4-[(furan-2- ylmethyl)-amino]-phenol	2,6-Difluoro-4-[(furan-2- ylmethyl)-amino]-phenol	4-(2-Trifluoromethyl- benzylamino)-benzene-1,3-diol	2,6-Difluoro-4-(2-trifluoromethyl- benzylamino)-phenol	N-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-propionamide
D H	HZ OH	HO OH	TZ OT U	JZ OF
1289	1290	1291	1292	1293

1294	D TY D TY	N-(3,5-Dichloro-4-hydroxy- phenyl)-2-(2-nitro-phenyl)- acetamide	C14H10Cl2N2O4	С, В	341.15	341.3
1295	TN TO	2-Benzo[1,3]dioxol-5-yl-N-(3,5-dichloro-4-hydroxy-phenyl)-acetamide	C15H11Cl2NO4	C, B	340.16	340.3
1296	HO DE TO	3-Methyl-but-2-enoic acid (3,5- dichloro-4-hydroxy-phenyl)-amide	C11H11Cl2NO2	. ບ	260.12	260.2
1297	TIN DE TO	Naphthalene-2-carboxylic acid (3,5-dichloro-4-hydroxy-phenyl)- amide	C17H11Cl2NO2	C, E	332.18	332.4
1298	TZ T	N-(3,5-Dichloro-4-hydroxy- phenyl)-benzamide	C13H9Cl2NO2	C, B	282.12	282.3

336.5
336.14
Q
C14H10Cl2F3NO
2,6-Dichloro-4-(2-trifluoromethyl-benzylamino)-phenol
CI CF3
1300

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or a pharmaceutical acceptable salt or prodrug thereof.

Even more preferred compounds according to the present invention are those mentioned in any of the tables herein and those further disclosed and/or characterized in the examples.

As used herein, each of the following terms, used alone or in conjunction with other terms, are preferably used in the following meaning (except where noted to the contrary):

The term "alkyl" refers to a saturated aliphatic radical containing from one to ten carbon atoms or a mono- or polyunsaturated aliphatic hydrocarbon radical containing from two to twelve carbon atoms, containing at least one double and triple bound, respectively. "Alkyl" refers to both branched and unbranched alkyl groups. Preferred alkyl groups are straight chain alkyl groups containing from one to eight carbon atoms. More preferred alkyl groups are straight chain alkyl groups containing from one to six carbon atoms and branched alkyl groups containing from three to six carbon atoms. It should be understood that any combination term using an "alk" or "alkyl" prefix refers to analogs according to the above definition of "alkyl". For example, terms such as "alkoxy", "alkylthio" refer to alkyl group linked to a second group via an oxygen or sulfur atom. "Alkanoyl" refers to an alkyl group linked to a carbonyl group (C=O). "Substituted alkyl" refers to alkyl groups straight or branched further bearing one or more substituents. One substituent also means monosubstituted and more substitutents mean poly-substituted. It should be understood that any combination term using a "substituted alkyl" prefix refers to analogs according to the above definition of "substituted alkyl". For example, a term such as "substituted alkylaryl" refers to substituted alkyl group linked to an aryl group.

The term "cycloalkyl" refers to the cyclic analog of an alkyl group, as defined above, optionally unsaturated and/or substituted. Preferred cycloalkyl groups are saturated cycloalkyl groups, more particularly those containing from three to eight carbon atoms, and even more preferably three to six carbon atoms. "Substituted cycloalkyl" refers to cycloalkyl groups further bearing one or more substituents. "Mono-unsaturated cycloalkyl" refers to cycloalkyl containing one double bond or one triple bond. "Poly-unsaturated cycloalkyl" refers to cycloalkyl containing at least two double bonds or two triple bonds or a combination of at least one double bond and one triple bond.

The term "alkenyl" refers to an unsaturated hydrocarbon group containing at least one carbon-carbon double bond, including straight-chain, branched-chain, and cyclic groups. Preferred alkenyl groups have one to twelve carbons. More preferred alkenyl groups have one to six carbons. "Substituted alkenyl" refers to alkenyl groups further bearing one or more substitutents.

The term "cycloalkenyl" refers to the cyclic analog of an alkenyl group, as defined above, optionally substituted. Preferred cycloalkenyl groups are containing from four to eight carbon atoms. "Substituted cycloalkenyl" refers to cycloalkenyl groups further bearing one or more substituents. "Mono-unsaturated cycloalkenyl" refers to cycloalkenyl containing one double bond. "Poly-unsaturated cycloalkenyl" refers to cycloalkenyl containing at least two double bonds.

The term "alkynyl" refers to an unsaturated hydrocarbon group containing at least one carbon-carbon triple bond, including straight-chain, branched-chain, and cyclic groups. Preferred alkynyl groups have one to twelve carbons. More preferred alkynyl groups have one to six carbons. "Substituted alkynyl" refers to alkynyl groups further bearing one or more substitutents.

The term "aryl" refers to aromatic groups having in the range of 6 to 14 carbon atoms and "substituted aryl" refers to aryl groups further bearing one or more substituents. It should be understood that any combination term using an "ar" or "aryl" prefix refers to analogs according to the above definition of "aryl". For example, a term such as "aryloxy" refers to aryl group linked to a second group via an oxygen.

Each of the above defined "alkyl", "cycloalkyl", and "aryl" shall be understood to include their halogenated analogs, whereby the halogenated analogs may comprise one or several halogen atoms. The halogenated analogs thus comprise any halogen radical as defined in the following.

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The term "halo" refers to a halogen radical selected from fluoro, chloro, bromo, iodo. Preferred halo groups are fluoro, chloro and bromo.

The term "heteroaryl" refers to a stable 5 to 8 membered, preferably 5 or 6 membered monocyclic or 8 to 11 membered bicyclic aromatic heterocycle radical. Each heterocycle consists of carbon atoms and from 1 to 4 heteroatoms selected from the group consisting of nitrogen, oxygen, sulfur. The heterocycle may be attached by any atom of the cycle, which preferably results in the creation of a stable structure. Preferred heteroaryl radicals as used herein include, for example, furanyl, thienyl, pyrrolyl, oxazolyl, thiazolyl, imidazolyl, pyrazolyl, isoxazolyl, isothiazolyl, oxadiazolyl, triazolyl, tetrazolyl, thiadiazolyl, pyridinyl, pyridazinyl, pyrimidinyl, pyrazinyl, indolizinyl, indolyl, isoindolyl, benzofuranyl, benzothienyl, indazolyl, benzimidazolyl, benzthiazolyl, benzoxazolyl, purinyl, quinolizinyl, quinolinyl, isoquinolinyl, cinnolinyl, phthalazinyl, quinazolinyl, quinoxalinyl, naphthridinyl, pteridinyl, carbazolyl, acridinyl, phenazinyl, phenothiazinyl and phenoxazinyl. "Substituted heteroaryl" refers to heteroaryl groups further bearing one or more substituents.

The term "heterocyclyl" refers to a stable 5 to 8 membered, preferably 5 or 6 membered monocyclic or 8 to 11 membered bicyclic heterocycle radical which may be either saturated or unsaturated, and is non-aromatic. Each heterocycle consists of carbon atom(s) and from 1 to 4 heteroatoms selected from the group consisting of nitrogen, oxygen and sulfur. The heterocycle may be attached by any atom of the cycle, which preferably results in the creation of a stable structure. Preferred heterocycle radicals as used herein include, for example, pyrrolinyl, pyrrolidinyl, pyrazolinyl, pyrazolidinyl, piperidinyl, morpholinyl, thiomorpholinyl, tetrahydropyranyl, indolinyl, azetidinyl, piperazinyl, pyranyl, thiopyranyl, tetrahydrothiopyranyl, tetrahydrofuranyl, hexahydropyrimidinyl, hexahydropyridazinyl, 1,4,5,6-tetrahydropyrimidin-2-ylamine, dihydro-oxazolyl, 1,2-thiazinanyl-1,1-dioxide, 1,2,6thiadiazinanyl-1,1-dioxide, isothiazolidinyl-1,1-dioxide and imidazolidinyl-2,4-dione. "Mono-unsaturated heterocyclyl" refers to heterocyclyl containing one double bond or one triple bond. "Poly-unsaturated heterocyclyl" refers to heterocyclyl containing at least two double bonds or two triple bonds or a combination of at least one double bond and one triple bond.

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"Substituted heterocyclyl" refers to heterocyclyl groups further bearing one or more substituents.

The terms "heterocyclyl", "heteroaryl" and "aryl", when associated with another moiety, unless otherwise specified, shall have the same meaning as given above. For example, "aroyl" refers to phenyl or naphthyl linked to a carbonyl group (C=O).

Each aryl or heteroaryl unless otherwise specified includes its partially or fully hydrogenated derivative. For example, quinolinyl may include decahydroquinolinyl and tetrahydroquinolinyl, naphthyl may include its hydrogenated derivatives such as tetrahydranaphthyl.

As used herein above and throughout this application, "nitrogen" or "N'and "sulfur" or "S" include any oxidized form of nitrogen and sulfur and the quaternized form of any basic nitrogen sulfoxide, sulfone, nitrone, N-oxide.

As used herein a wording defining the limits of a range of length such as e. g. "from 1 to 5" means any integer from 1 to 5, i. e. 1, 2, 3, 4 and 5. In other words, any range defined by two integers explicitly mentioned is meant to comprise any integer defining said limits and any integer comprised in said range.

As used herein the term substituted shall mean that one or more H atom of the group or compound which is substituted, is replaced by a different atom, a group of atoms, a molecule or a molecule moiety. Such atom, group of atoms, molecule or molecule moiety is also referred to herein as substituent.

The substituent can be selected from the group comprising hydroxy, alkoxy, mercapto, cycloalkyl, heterocyclic, aryl, heteroaryl, aryloxy, halogen, trifluoromethyl, difluoromethyl, cyano, nitrone, amino, amido, -C(O)H, acyl, oxyacyl, carboxyl, carbamate, sulfonyl, sulphonamide and sulfuryl. Any of the substituents may be substituted itself by any of the aforementioned substituents. This applies preferably to cycloalkyl, heterocylic, aryl, heteroaryl and aryloxy. It is also preferred that alkoxy and mercapto are those of a lower alkyl

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group. It is to be acknowledged that any of the definition provided herein also applies to any substituent.

A substituent can also be any of R^a, R^b, R^c, R^d, R^e, R^f, and R^g and/or any of R₁ to R₂₁. It is also within the present invention that any substitutent may in turn be substituted by a substituent. A group, structure, moiety or the like which is substituted may comprise several substituents which may either be different or the same.

As used herein =T can mean in any embodiment of the various aspects of the present invention that with =T is selected from electron withdrawing groups, whereby preferably the electron withdrawing groups are selected from =O, =N-R^e, =N-CN, =N-NO₂ and =CH-NO₂, and =S,

It is within the present invention that any thiourea moieties and derivates therefrom, particularly those described herein, can, in principle be replaced by a cyanoguanidine moiety or residue and respective derivates therefrom as described in J. Med. Chem 1977, 20, 901 – 906. In Addition to being weakly basic cyanoguanidine and thiourea are also weakly acidic and both are therefore neutral and weakly amphoteric compounds. Cyanoguanidine is also similar to thiourea in its geometry since both are planar structures with almost identical C-N bond lengths and bond angles. Another property common to thioureas and cyanoguanidines is conformational isomerism resulting from restricted C-N bond rotation. Cyanoguanidine and thiourea are similar in their hydrophilicity and hydrogen-bonding properties; they have comparably low octanol-water partition coefficients (P) and are both reasonably soluble in water.

As used herein in connection with an embodiment of the various aspects of the present invention the term "wherein R₁ and R₂, R₂ and R₃, R₃ and R₄, R₁ and R₃, R₁ and R₄, or R₂ and R₄ may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members" shall mean that any of the two residues R, such as, for example, R₁ and R₂ or R₂ and R₃, are linked to each through a covalent bond, a non-covalent bond or any combination thereof. The formation of the ring may be the result of one or several of this kind of bonds. It is to be understood that the molecule may comprise one or more of those rings formed by two residues R.

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In a preferred embodiment wherein R₁ and R₂, R₂ and R₃, R₃ and R₄, R₁ and R₃, R₁ and R₄, or R₂ and R₄ linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 members, R1, R2, R3 and R4 are each and independently selected from the group comprising H, OR6, SR7, NR8R9, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted heterocyclyl, substituted heterocyclyl, substituted aryl, alkylcycloalkyl, aryl, alkylheterocyclyl, heteroaryl, heteroaryl, substituted alkylheterocyclyl, substituted alkylheteroaryl and substituted alkylheteroaryl;

The ring may be cycloalkyl, heterocyclyl, aryl, or heteroaryl. The cycloalkyl or heterocyclyl ring can be mono-unsaturated or poly-unsaturated. The ring can be substituted by one or more substituents as defined herein

As used herein in connection with an embodiment of the various aspects of the present invention the term "each and independently selected from a group" or "are independently from each other selected from the group" refers to two or more atoms, groups, substituents, moieties or whatsoever and describes that the single atom, group etc. mentioned can be selected from the group. The wording used is a truncation which avoids unnecessary repetition as otherwise for each of the atoms, groups etc. the same group definition would have to be repeated.

As used herein in connection with an embodiment of the various aspects of the present invention the term "each and individually absent" refers to two or more atoms, groups, substituents, moieties or whatsoever and describes that the single atom, group etc. mentioned can be absent regardless whether any of the other atoms, groups etc. mentioned is absent. The wording used is a truncation which avoids unnecessary repetition as otherwise for each of the atoms, groups etc. the fact that it may be absent in an embodiment of the invention would have to be repeated.

In connection with the present invention some groups such as, e.g.,  $-(CR^aR^b)$ — or  $-(CR^fR^g)$ —are repeated, i.e. are repeatedly present in a compound according to the present invention. Typically such repetition occurs in such a manner that, e.g.,  $-(CR^aR^b)$ — is repeated one or

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several times. In case, e.g.,  $-(CR^aR^b)$ — is repeated one time which means that there are two consecutive groups of  $-(CR^aR^b)$ —, these two forms of  $-(CR^aR^b)$ — can be either the same or they may be different in a different embodiment which means that either  $R^a$  or  $R^b$  or both of them are different between said two  $-(CR^aR^b)$ — groups. If there are three or more of these groups such as , e.g.,  $-(CR^aR^b)$ —, it is possible that all of them are different or only some or different whereas others are the same in the sense defined above. Any permutation for the arrangement for such identical or different groups is within the present invention.

The same applies to the design and arrangement of the spacer -M1-L1-K-L2-M2-.

In connection with any of the compounds according to the present invention and more particularly in connection with the compounds according to formulae VI to XIII and XIX to XXVI it is to be noted that the formation of a ring structure through E between the cyclic moiety A such as the phenol moiety and the spacer X can occur between the cyclic moiety A such as the phenol moiety and any of the spacer moieties -M1-L1-K-L2-M2-, regardless whether they are of a linear or any of the cyclic structures themselves. It is therefore within the present invention that in case of a repetition of the above described spacer moiety -M1-L1-K-L2-M2- the ring formation can either occur at the -M1-L1-K-L2-M2- moiety which is next or closest to the ring as represented in the respective formulae, or at the or any of the further -M1-L1-K-L2-M2- moieties present in the particular compound.

As used herein in connection with an embodiment of the various aspects of the present invention the term C=T shall represent a C atom having a double bond with T which represents certain atoms, groups, substituents, moieties or the like as further defined herein.

It is within the present invention that the features of the various embodiments of the present invention can be realized either alone or in combination with the features of any other embodiment(s) of the present invention. Thus any combination of an/the individual feature or the combination of features of an embodiment of the present invention with an/the individual feature(s) or the combination of features of any other embodiment(s), either alone or in combination with other embodiments, shall be disclosed by the present specification.

As used herein in connection with an embodiment of the various aspects of the present invention the term referring to a group, substituent, moiety, spacer or the like specifying that it "can be inserted in any orientation into any of the preceding formulae" means that the group etc. can be attached to another atom, group, substitutent, moiety spacer or the like of any of the compounds according to the present invention or any of the formulae disclosed herein via any of its ends an in particular through any of the atoms arranged at the ends of said group, substituent, moiety, spacer or the like.

In a further aspect the present invention is related to the use of a compound according to any of the aspects of the present invention as an inhibitor to or for a rotamase.

In an embodiment the rotamase regulates a part of the cell cycle.

In a preferred embodiment the rotamase regulates a part of the cell cycle, whereby preferably the part of the cell cycle is mitosis.

In an even more preferred embodiment the rotamase is a mammalian rotamase, preferably a human rotamase, more preferably hPin1.

In a further aspect the present invention is related to the use of the compounds according to the present invention as a pharmaceutical or in a pharmaceutical composition or for the manufacture of such pharmaceutical composition which is preferably for the prophylaxis and/or treatment of a disease, whereby the disease involves a rotamase, whereby the rotamase is a mammalian rotamase, preferably a human rotamase, more preferably hPin1.

In connection with the further aspect of the present invention related to the use of any of the aforementioned compounds according to the present invention as an inhibitor to rotamases the following will be acknowledged by the one skilled in the art. In view of the characteristics of the compounds according to the present invention to be active as an inhibitor of (a) rotamase(s), it is sufficient that the respective compound is at least suitable to inhibit at least one rotamase. The compounds according to the present invention which may be used as inhibitors, are also referred to as rotamase inhibitors herein.

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Rotamases as such are known in the art and, for example, described in the introductory part of this specification which is incorporated by reference. Rotamases as used herein shall mean cyclophilins, FK-506 binding proteins and the rotamases of the Pin1/parvulin class. The Pin1/parvulin class includes Pins 1 to 3, PinL/parvulin, dodo, and Es1/Pft1. Suitable assays to determine whether a compound is suitable to inhibit a rotamase are known to the one skilled in the art and also described in the present examples. Basically, a rotamase is provided the activity of which or non-activity of which may be determined. A candidate inhibitor, i. e. a compound which is to be tested whether it is active as an inhibitor to rotamase, is added to the rotamase and tested whether upon the addition and/or influence of the candidate inhibitor the activity of the rotamase is changed relative to the activity without candidate rotamase inhibitor. If the rotamase activity is decreased by the candidate rotamase inhibitor, said candidate rotamase inhibitor is a rotamase inhibitor according to the present invention.

In another aspect of the present invention the compounds according to the present invention may be used in a method for inhibiting a rotamase. In such case a rotamase is provided and a candidate rotamase inhibitor is added thereto whereupon the activity of rotamase is decreased. Optionally, such decrease in rotamase activity is measured. The techniques used theretofore are basically the same as outlined in connection with the use of the compounds according to the present invention as rotamase inhibitors.

The compounds according to the present invention are preferably reversible rotamase inhibitors.

By "reversible" herein is meant that the inhibitor binds non-covalently to the enzyme, and is to be distinguished from irreversible inhibition. See Walsh, Enzymatic Reaction Mechanisms, Freeman & Co., N.Y., 1979. "Reversible" in this context is a term understood by those skilled in the art. Preferably the rotamase inhibitors according to the present invention are competitive inhibitors, that is, they compete with substrate in binding reversibly to the enzyme, with the binding of inhibitor and substrate being mutually exclusive.

In a preferred embodiment of the compounds according to the present invention being active as a rotamase inhibitor, the dissociation constant for inhibition of a rotamase with the inhibitor, generally referred to and characterized by those in the art as  $K_i$ , is at most about 100

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μM. By the term "binding constant" or "dissociation constant" or grammatical equivalents herein is meant the equilibrium dissociation constant for the reversible association of inhibitor with enzyme. The dissociation constants are defined and determined as described below. The determination of dissociation constants is known in the art. For example, for reversible inhibition reactions such as those of the present invention, the reaction scheme is as follows:

E+I 
$$\frac{k_1}{k_2}$$
 E*I (Equation 1)

The enzyme (E) and the inhibitor (I) combine to give an enzyme-inhibitor complex (E*I). This step is assumed to be rapid and reversible, with no chemical changes taking place; the enzyme and the inhibitor are held together by non-covalent forces. In this reaction,  $k_1$  is the second order rate constant for the formation of the E*I reversible complex.  $k_2$  is the first order rate constant for the dissociation of the reversible E*I complex. In this reaction,  $K_1 = k_2/k_1$ .

The measurement of the equilibrium constant  $K_i$  proceeds according to techniques well known in the art, as described in the examples. For example, assays generally use synthetic chromogenic or fluorogenic substrates. The respective  $K_i$  values may be estimated using the Dixon plot as described by Irwin Segel in Enzyme Kinetics: Behavior and analysis of rapid equilibrium and steady-state enzyme systems, 1975, Wiley-Interscience Publication, John Wiley & Sons, New York, or for competitive binding inhibitors from the following calculation:

$$1-(v_i/v_o)=[I]/[I]+K_i (1+([S]/K_m)))$$
 (Equation 2)

wherein  $v_0$  is the rate of substrate hydrolysis in the absence of inhibitor, and  $v_i$  is the rate in the presence of competitive inhibitor.

It is to be understood that dissociation constants are a particularly useful way of quantifying the efficiency of an enzyme with a particular substrate or inhibitor, and are frequently used in the art as such. If an inhibitor exhibits a very low  $K_i$  value, it is an efficient inhibitor. Accordingly, the rotamase inhibitors of the present invention have dissociation constants,  $K_i$ ,

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of at most about 100  $\mu$ M. Preferably, the rotamase inhibitors according to the present invention exhibit dissociation constants of at most about 10  $\mu$ M, more preferably about 1  $\mu$ M, most preferably of at most about 100 nM.

The rotamase inhibitors of the present invention may be easily screened for their inhibitory effect. The inhibitor is first tested against different classes of rotamases for which the targeting group of the inhibitor was chosen, as outlined above. The activity of rotamases is typically measured by using a protease coupled assay with chromogenic substrates and conformer specific proteases. Basically, upon the conformer specific protease activity the chromogenic substrate is converted into a compound which has an absorption characteristic which is different from the starting chromogenic substrate and may thus be selectively measured. This reaction is accelerated in presence of the rotamase and decelerated in the presence of rotamase-inhibitors. Alternatively, many rotamases and their corresponding chromogenic substrates are commercially available. Thus, a variety of rotamases are routinely assayed with synthetic chromogenic substrates in the presence and absence of the rotamase inhibitor, to confirm the inhibitory action of the compound, using techniques well known in the art. The effective inhibitors are then subjected to kinetic analysis to calculate the K_i values, and the dissociation constants determined.

If a compound inhibits at least one rotamase, it is a rotamase inhibitor for the purposes of the present invention. Preferred embodiments of the rotamase inhibitors according to the present invention are compounds and inhibitors, respectively, that exhibit the correct kinetic parameters Ki below 100  $\mu$ M against the targeted rotamases.

In a further aspect of the present invention any of the compounds used as rotamase inhibitors or as a medicament may be labelled.

By a "labelled rotamase inhibitor" herein is meant a rotamase inhibitor that has at least one element, isotope or chemical compound attached to enable the detection of the rotamase inhibitor or the rotamase inhibitor bound to a rotamase. In general, labels as used herein, fall into three classes: a) isotopic labels, which may be radioactive or heavy isotopes; b) immune labels, which may be antibodies or antigens; and c) colored or fluorescent dyes. The labels

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may be incorporated into the rotamase inhibitor at any position. Examples of useful labels include ¹⁴C, ¹³C, ¹⁵N, ³H, biotin, and fluorescent labels as are well known in the art.

In a further aspect the compounds according to the present invention, particularly those having rotamase inhibitory activity, may be used for removing, identifying and/or inhibiting contaminating rotamases in a sample.

Therefore, the rotamase inhibitors of the present invention are, for example, added to a sample where the catalytic activity by contaminating rotamases is undesirable. Alternatively, the rotamase inhibitors of the present invention may be bound to a chromatographic support, using techniques well known in the art, to form an affinity chromatography column. A sample containing an undesirable rotamase is run through the column to remove the rotamase. Alternatively, the same methods may be used to identify new rotamases. In doing so, a new rotamase contained in a sample may bind to the rotamase inhibitor bound to the chromatographic support and upon elution, preferably a specific elution, from said chromatographic support, characterized and compared to other rotamase activities with regard to, among others, specificities. The characterization of the rotamase as such is known to the one skilled in the art.

In a further aspect the present invention is related to a pharmaceutical composition comprising a compound according to any of the aspects of the present invention and a pharmaceutically acceptable carrier, diluent or excipient.

In an embodiment the composition comprises a further pharmaceutically active compound, preferably such further pharmaceutically active compound is a chemotherapeutic agent.

In a preferred embodiment of the composition the compound is present as a pharmaceutically acceptable salt or a pharmaceutically active solvate.

In an even more preferred embodiment the pharmaceutically active compound is either alone or in combination with any of the ingredients of the composition present in a multitude of individualized dosages and/or administration forms.

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The use of the compounds according to the present invention for the manufacture of a medicament is based on the fact that the compounds according to the present invention are inhibitors of rotamases and rotamases in turn have been identified in both procaryotic and eucaryotic cells such as in bacteria, fungi, insect and mammalian cells. In this cellular environment rotamases are known to have an impact on cell proliferation and mitosis, respectively. Because of this, rotamase inhibitors may be used for the treatment of a wide variety of disorders involving cell cycle regulation, both procaryotic and eucaryotic cell cycle regulation. The term "treatment" as used herein comprises both treatment and prevention of a disease. It also comprises follow-up treatment of a disease. Follow-up treatment is realized upon a treatment of a disease using compounds preferably different from the one according to the present invention. For example, after stimulating the growth of a cell, tissue or the like by the application of a respective compound such as, e. g., erythropoietin, it might be necessary to stop an overshooting reaction of cell proliferation which may be obtained using the compounds according to the present invention.

In a further aspect the present invention is related to the use of the compounds according to the present invention as a medicament and for the manufacture of a medicament, respectively. It is to be understood that any of the compounds according to the present invention can be used for the treatment of or for the manufacture of a medicament for the treatment of any of the diseases disclosed herein, irrespective of the mode of action or the causative agent involved as may be specified herein. Of Course, it may particularly be used for any form of such disease where the particular causative agent is involved. Causative agent as used herein also means any agent which is observed in connection with the particular disease described and such agent is not necessarily causative in the sense that is causes the observed diseases or diseased condition.

In an embodiment the medicament is for the treatment or prevention of a disease, whereby the disease involves an undesired cell proliferation.

This use of the compounds according to the present invention is based on the fact that the compounds according to the present invention are suitable to inhibit undesired cell proliferation. Undesired cell proliferation comprises the undesired cell proliferation of procaryotic cells as well as undesired cell proliferation of eucaryotic cells. The term undesired

cell proliferation also covers the phenomenon of abnormal cell proliferation, abnormal mitosis and undesired mitosis. Abnormal cell proliferation means any form of cell proliferation which occurs in a manner different from the normal cell proliferation. Normal cell proliferation is a cell proliferation observed under normal circumstances by the majority of cells and organisms, respectively. The same basic definition applies to abnormal mitosis.

More particularly, undesired cell proliferation and undesired mitosis mean a proliferation and a mitosis, respectively, which may be either a normal or an abnormal cell proliferation, however, in any case it is not a cell proliferation or mitosis which is desired. Desired may thus be defined by an individual such as a human being and in particular a physician, and defined within certain boundaries whereby the boundaries as such may reflect the extent of proliferation and mitosis, respectively, observed under usual conditions or in the majority of cells and organisms, respectively, or may be arbitrarily fixed or defined. Cell proliferation as used herein refers preferably to the proliferation of cells forming the organism to be treated or to which a compound according to the present invention shall be administered which is also referred to herein as the first organism. Cell proliferation as used herein also means the proliferation of cells which are different from the cells forming a first organism or species but are the cells forming a second organism or second species. Typically, the second organism enters in or has a relationship with the first organism. Preferably, the first organism is a human being or an animal or plant, also referred to herein as patient, and the second organism is a parasite and pathogen, respectively, to said first organism. Mitosis as used herein, preferably means the cell division of cells being subject to said cell proliferation whereby even more preferably mitosis is the process of cell division whereby a complete set of chromosomes is distributed to the daughter cells.

Without wishing to be bound by any theory, it seems that the compounds according to the present invention act on cells and thus influence their proliferation and mitosis, respectively, by being inhibitors to some enzymatic activity. Preferably, the inhibition is reversible. This activity is shown by the compounds according to the present invention with regard to bacteria, fungi, insect and mammalian cells.

Because of this, the compounds according to the present invention may be used for the treatment of a wide variety of disorders involving cell cycle regulation, both procaryotic and

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eucaryotic cell cycle regulation. The term "treatment" as used herein comprises both treatment and prevention of a disease. It also comprises follow-up treatment of a disease. Follow-up treatment is realized upon a treatment of a disease using compounds preferably different from the one according to the present invention. For example, after stimulating the growth of a cell, tissue or the like by the application of a respective compound such as, e. g., erythropoietin, it might be necessary to stop an overshooting reaction of cell proliferation which may be obtained using the compounds according to the present invention.

By "reversible" herein is meant that the inhibitor binds non-covalently to the respective enzyme, and is to be distinguished from irreversible inhibition. See Walsh, Enzymatic Reaction Mechanisms, Freeman & Co., N.Y., 1979. "Reversible" in this context is a term understood by those skilled in the art. Preferably the compounds according to the present invention are competitive inhibitors, that is, they compete with substrate in binding reversibly to the enzyme, with the binding of inhibitor and substrate being mutually exclusive.

In a preferred embodiment of the compounds according to the present invention the dissociation constant for inhibition of the enzyme(s) with the inhibitor, i. e. the compound according to the present invention, generally referred to and characterized by those in the art as  $K_i$ , is at most about 100  $\mu$ M. By the term "binding constant" or "dissociation constant" or grammatical equivalents herein is meant the equilibrium dissociation constant for the reversible association of inhibitor with enzyme. The dissociation constants are defined and determined as described below. The determination of dissociation constants is known in the art. For example, for reversible inhibition reactions such as those of the present invention, the reaction scheme is as follows:

E+I 
$$\stackrel{k_1}{=}$$
 E*I (Equation 1)

The enzyme (E) and the inhibitor (I) combine to give an enzyme-inhibitor complex (E*I). This step is assumed to be rapid and reversible, with no chemical changes taking place; the enzyme and the inhibitor are held together by non-covalent forces. In this reaction,  $k_1$  is the

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second order rate constant for the formation of the E*I reversible complex.  $k_2$  is the first order rate constant for the dissociation of the reversible E*I complex. In this reaction, Ki = $k_2/k_1$ .

The measurement of the equilibrium constant K_i proceeds according to techniques well known in the art. For example, assays generally use synthetic chromogenic or fluorogenic substrates. The respective K_i values may be estimated using the Dixon plot as described by Irwin Segel in Enzyme Kinetics: Behavior and analysis of rapid equilibrium and steady-state enzyme systems, 1975, Wiley-Interscience Publication, John Wiley & Sons, New York, or for competitive binding inhibitors from the following calculation:

$$1-(\nu_i/\nu_o) = [I]/[I] + K_i (1+([S]/K_m))) \quad \text{(Equation 2)}$$

wherein  $v_0$  is the rate of substrate hydrolysis in the absence of inhibitor, and  $v_i$  is the rate in the presence of competitive inhibitor.

The compounds according to the present invention may be easily screened for their efficacy in relation to the various uses disclosed herein

By a "labelled compound according to the present invention" herein is meant a compound according to the present invention that has at least one element, isotope or chemical compound attached to enable the detection of the compound or the compound bound to a target such as an enzyme. In general, labels as used herein, fall into three classes: a) isotopic labels, which may be radioactive or heavy isotopes; b) immune labels, which may be antibodies or antigens; and c) colored or fluorescent dyes. The labels may be incorporated into the compound at any position. Examples of useful labels include ¹⁴C, ¹³C, ¹⁵N, ³H, biotin, and fluorescent labels as are well known in the art.

As used herein, the term "disease" describes any disease, diseased condition or pathological condition. Such disease may also be defined as abnormal condition. Also, in case of a pathogen, disease means a condition where a pathogen or an unwanted organism is present or present in a concentration or compartment where it is undesired and thus subject to reduction in numbers, removal, elimination and/or destruction by using the compounds according to the present invention.

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The compounds according to the present invention may be used as a medicament and for the manufacture of a medicament, respectively, whereby the medicament is for the treatment of cell proliferative disorders and any of the diseases specified herein. Cell proliferated disorders as used herein, typically involve an abnormal cell proliferation, an undesired cell proliferation, an abnormal mitosis and/or an undesired mitosis.

Cell proliferative disorders contemplated for treatment using the compounds according to the present invention and for the methods disclosed herein include also disorders characterized by unwanted or undesired, inappropriate or uncontrolled cell growth. Preferably, the disease is selected from the group comprising neurodegenerative diseases, stroke, inflammatory diseases, immune based disorders, infectious diseases, heart diseases, fibrotic disorders, cardiovascular diseases and cell proliferative diseases. Rotamases comprise families of ubiquitous and highly conserved enzymes who have been reported to play important roles in biological processes like protein folding, proteolysis, protein dephosphorylation, peptide transport function, cell cycle regulation, protein synthesis. Furthermore various isomerases have been shown to have regulatory functions as stable or dynamic part of heterooligomeric complexes containing physiologically relevant proteins e.g. hormone receptors, ion channels, kinases, and growth factor receptors.

Preferably, the neurodegenerative disease is selected from the group comprising Alzheimer's disease, Huntington's disease, Parkinson's disease, peripheral neuropathy, progressive supranuclear palsy, corticobasal degeneration, frontotemporal dementia, synucleinopathies, multiple system atrophy, amyotrophic lateral atrophy, prion diseases and motor neuron diseases.

The compounds according to the present invention are additionally useful in inhibiting cell cycle (mitosis) or cell division in pathogenic organisms and are, therefore, useful for treating infectious diseases.

In a preferred embodiment the infectious is selected from the group comprising fungal, viral, bacterial and parasite infection.

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Fungal infections contemplated for treatment using the compounds and methods according to the present invention include systemic fungal infections, dermatophytoses and fungal infections of the genito-urinary tract. Fungal infections, preferably systemic fungal infections, include those caused by Histoplasma, Coccidioides, Cryptococcus, Blastomyces, Paracoccidioides, Aspergillus, Nocardia, Sporothrix, Rhizopus, Absidia, Mucor, Hormodendrum, Phialophora, Rhinosporidium, and the like. Dermatophyte infections include those caused by Microsporum, Trichophyton, Epidermophyton, Candida, Pityrosporum, and the like. Fungal disorders of the genito-urinary tract include infections caused by Candida, Cryptococcus, Aspergillus, Zygomycodoides, and the like. Infection by such organisms causes a wide variety of disorders such as ringworm, thrush or candidiasis, San Joaquin fever or Valley fever or coccidiodomycosis, Gilchrist's disease or blastomycosis, aspergillosis, cryptococcosis, histioplasmosis, paracoccidiomycosis, zygomycosis, mycotic keratitis, nail hair and skin disease, Lobo's disease, lobomycosis, chromoblastomycosis, mycetoma, and the like. These infections can be particularly serious, and even fatal, in patients with a depressed immune system such as organ transplant recipients and persons with acquired immunodefficiency syndrome (AIDS). Insofar a patient group which can be treated using the inhibitors according to the present invention are persons with AIDS, particularly those suffering from any of the infectious diseases described herein.

In a further embodiment the bacterial infection is selected from the group comprising infections caused by both Gram-positive and Gram-negative bacteria, including infections caused by Staphylococcus, Clostridium, Streptococcus, Enterococcus, Diplococcus, Hemophilus, Neisseria, Erysipelothricosis, Listeria, Bacillus, Salmonella, Shigella, Escherichia, Klebsiella, Enterobacter, Serratia, Proteus, Morganella, Providencia, Yersinia, Camphylobacter, Mycobacteria, Helicobacter, Legionalla, Nocardia and the like.

In a preferred embodiment the bacterial infection causes a wide variety of diseases. Said disorders are selected, among others, from the group comprising pneumonia, diarrhea, dysentery, anthrax, rheumatic fever, toxic shock syndrome, mastoiditis, meningitis, gonorrhea, typhoid fever, brucellis, Lyme disease, gastroenteritis, tuberculosis, cholera, tetanus and bubonic plague.

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In another embodiment the disease is a viral infection, more particularly a viral infection caused by a virus selected from the group comprising retrovirus, HIV, Papilloma virus, Polio virus, Epstein-Barr, Herpes virus, Hepatitis virus, Papova virus, Influenza virus, Rabies, JC, encephalitis causing virus, hemorrhagic fever causing virus such as Ebola Virus and Marburg Virus.

In a further embodiment the parasite infection is selected from the group comprising infections caused by Trypanosoma, Leishmania, Trichinella, Echinococcus, Nematodes, Classes Cestoda, Trematoda, Monogenea, Toxoplasma, Giardia, Balantidium, Paramecium, Plasmodium or Entamoeba.

The disease may further be a cell proliferative disorder which preferably is selected from the group characterized by unwanted, inappropriate or uncontrolled cell growth. Particular examples include cancer, fibrotic disorders, non-neoplastic growths. The neoplastic cell proliferative disorder is preferably selected from the group comprising solid tumors, and hematopoeitic cancers such as lymphoma and leukemia.

More preferably, the solid tumor is selected from the group comprising carcinoma, sarcoma, osteoma, fibrosarcoma, and chondrosarcoma.

More preferably, the cell proliferative disorder is selected from the group comprising breast cancer, prostate cancer, colon cancer, brain cancer, lung cancer, pancreatic cancer, gastric cancer, bladder cancer, kidney cancer and head and neck cancer. Preferably, the lung cancer is non-small lung cancer and small lung cancer.

In case the disease is a non-neoplastic cell proliferative disorder, it is preferably selected from the group comprising fibrotic disorder. Preferably, the fibrotic disorder is fibrosis.

The disease may also be a non-neoplastic cell proliferative disorder which is selected from the group comprising prostatic hypertrophy, preferably benign prostatic hypertrophy, endometriosis, psoriasis, tissue repair and wound healing.

Fibrotic disorders which may be treated using the compounds according to the present invention are generally characterized by inappropriate overproliferation of non-cancerous fibroblasts. Examples thereof include fibromyalgia, fibrosis, more particularly cystic, hepatic, idopathic pulmonary, and pericardial fibrosis and the like, cardiac fibromas, fibromuscular hyperplasia, restenosis, atherosclerosis, fibromyositis, and the like.

In another embodiment the immune based and/or inflammatory disease is an autoimmune disease or autoimmune disorder. In a further embodiment, the immune based and/or inflammatory disease is selected from the group comprising rheumatoid arthritis, glomerulonephritis, systemic lupus erythematosus associated glomerulonephritis, irritable bowel syndrome, bronchial asthma, multiple sclerosis, pemphigus, pemphigoid, scleroderma, myasthenia gravis, autoimmune haemolytic and thrombocytopenic states, Goodpasture's syndrome, pulmonary hemorrhage, vasculitis, Crohn's disease, and dermatomyositis.

In a further preferred embodiment the immune based and/or inflammatory disease is an inflammatory condition.

In a still further embodiment the immune based and/or inflammatory disease is selected from the group comprising inflammation associated with burns, lung injury, myocardial infarction, coronary thrombosis, vascular occlusion, post-surgical vascular reocclusion, artherosclerosis, traumatic central nervous system injury, ischemic heart disease and ischemia-reperfusion injury, acute respiratory distress syndrome, systemic inflammatory response syndrome, multiple organ dysfunction syndrome, tissue graft rejection and hyperacute rejection of transplanted organs.

It is also within the present invention that the compounds according to the present invention may be used for the treatment of a patient suffering from a disease or diseased condition as defined above. Such treatment comprises the administration of one or several of the compounds according to the present invention or a medicament or pharmaceutical composition described herein.

Toxicity and therapeutic efficacy of a compound can be determined by standard pharmaceutical procedures in cell culture or experimental animals. Cell culture assays and

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animal studies can be used to determine the  $LD_{50}$  (the dose lethal to 50% of a population) and the  $ED_{50}$  (the dose therapeutically effective in 50% of a population). The dose ratio between toxic and therapeutic effects is the therapeutic index, which can be expressed as the ratio  $LD_{50}/ED_{50}$ . Compounds which exhibit large therapeutic indices are preferred. The data obtained from these cell culture assays and animal studies can be used in formulating a range of dosages suitable for use in humans. The dosage may vary within this range depending upon a variety of factors, e.g., the dosage form employed, the route of administration utilized, the condition of the subject, and the like

For any compound according to the present invention, the therapeutically effective dose can be estimated initially from cell culture assays by determining an IC₅₀ (i.e., the concentration of the test substance which achieves a half-maximal inhibition of cell proliferation). A dose can then be formulated in animal models to achieve a circulating plasma concentration range that includes the IC₅₀ as determined in cell culture. Such information can be used to more accurately determine useful doses in humans. Levels in plasma may be measured, for example by HPLC or LC/MS.

It should be noted that the attending physician would know how to and when to terminate, interrupt, or adjust administration due to toxicity, to organ dysfunction, and the like. Conversely, the attending physician would also know to adjust treatment to higher levels if the clinical response were not adequate (precluding toxicity). The magnitude of an administered dose in the management of the disorder of interest will vary with the severity of the condition to be treated, with the route of administration, and the like. The severity of the condition may, for example, be evaluated, in part, by standard prognostic evaluation methods. Further, the dose and perhaps dose frequency will also vary according to the age, body weight, and response of the individual patient. Typically, the dose will be between about 1-10 mg/kg of body weight. About 1 mg to about 50 mg will preferably be administered to a child, and between 25 mg and about 1000 mg will preferably be administered to an adult.

A program comparable to that discussed above may be used in veterinary medicine. The exact dose will depend on the disorder to be treated and will be ascertainable by one skilled in the art using known techniques.

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Depending on the specific conditions to be treated, such compounds may be formulated and administrated systemically or locally. Techniques for formulation and administration may be found in "Remington's Pharmaceutical Sciences", 1990, 18th ed., Mack Publishing Co., Easton, PA. The administration of a compound according to the present invention can be done in a variety of ways, including, but not limited to, orally, subcutaneously, intravenously, intranasally, transdermally, intraperitoneally, intramuscularly, intrapulmonary, vaginally, rectally, or intraocularly, just to name a few. In some instances, for example, in the treatment of wounds and inflammation, the compound according to the present invention may be directly applied as a solution or spray.

In a further aspect the present invention is related to a medicament or a pharmaceutical composition comprising at least one active compound and at least one pharmaceutically acceptable carrier, excipient or diluent. As used herein, the active compound is a compound according to the present invention, a pharmaceutically salt or base thereof or a prodrug thereof, if not indicated to the contrary.

For injection, compounds of the invention may be formulated in aqueous solution, preferably in physiologically compatible buffers such as Hank's solution, Ringer's solution, or physiologically saline buffer. For transmucosal administration, penetrants appropriate to the barrier to be permeated are used in the formulation. Such penetrants are generally known in the art.

The use of pharmaceutical acceptable carriers to formulate the compounds according to the present invention into dosages or pharmaceutical compositions suitable for systemic administration is within the scope of the present invention. With proper choice of carrier and suitable manufacturing practice, the compositions of the present invention, in particular those formulated as solutions, may be administered parenterally, such as by intravenous injection. The compounds can be readily formulated using pharmaceutically acceptable carriers well known in the art into dosages suitable for oral administration. Such carriers enable the compounds according to the present invention to be formulated as tablets, pills, capsules, dragees, liquids, gels, syrups, slurries, suspensions and the like, for oral ingestion by a subject to be treated.

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Compounds according to the present invention or medicaments comprising them, intended to be administered intracellularly may be administered using techniques well known to those of ordinary skill in the art. For example, such agents may be encapsulated into liposomes, then administered as described above. Liposomes are spherical lipid bilayers with aqueous interiors. All molecules present in an aqueous solution at the time of liposome formation are incorporated into the aqueous interior. The liposomal contents are both protected from the external microenvironment and, because liposomes fuse with cell membranes, are efficiently delivered into the cell cytoplasm. Delivery systems involving liposomes are disclosed in International Patent Publication No. WO 91/19501, as well as U.S. Patent No. 4,880,635 to Janoff et al. The publications and patents provide useful descriptions of techniques for liposome drug delivery and are incorporated by reference herein in their entirety.

Pharmaceutical compositions comprising a compound according to the present invention for parenteral administration include aqueous solutions of the active compound(s) in water-soluble form. Additionally, suspensions of the active compounds may be prepared as appropriate oily injection suspensions. Suitable lipophilic solvents or vehicles include fatty oils such as sesame oil or castor oil, or synthetic fatty acid esters, such as ethyl oleate or triglycerides, or liposomes. Aqueous injections suspensions may contain compounds which increase the viscosity of the suspension, such as sodium carboxymethyl cellulose, sorbitol, dextran, or the like. Optionally, the suspension may also contain suitable stabilizers or agents which increase the solubility of the compounds to allow for the preparation of highly concentrated solutions.

Pharmaceutical compositions comprising a compound according to the present invention for oral use can be obtained by combining the active compound(s) with solid excipient, optionally grinding the resulting mixture, and processing the mixture of granules, after adding suitable auxiliaries, if desired, to obtain tablets or dragee cores.

Suitable excipients are, in particular, fillers such as sugars, including lactose, sucrose, mannitol, sorbitol, and the like; cellulose preparations, such as, for example, maize starch wheat starch, rice starch, potato starch, gelatin, gum tragacanth, methyl cellulose, hydroxypropylmethyl cellulose, sodium carboxymethyl cellulose, polyvinylpyrrolidone (PVP) and the like, as well as mixtures of any two or more thereof. If desired, disintegrating agents

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may be added, such as cross-linked polyvinyl pyrrolidone, agar, alginic acid or a salt thereof such as sodium alginate, and the like.

Dragee cores as a pharmaceutical composition comprising a compound according to the present invention are provided with suitable coatings. For this purpose, concentrated sugar solutions may be used, which may optionally contain gum arabic, talc, polyvinyl pyrrolidone, carbopol gel, polyethylene glycol, titanium dioxide, lacquer solutions, suitable organic solvents or solvent mixtures, and the like. Dyestuffs or pigments may be added to the tablets or dragee coatings for identification or to characterize different combinations of active compound doses.

Pharmaceutical preparations comprising a compound according to the present invention which can be used orally include push-fit capsules made of gelatin, as well as soft, sealed capsules made of gelatin and a plasticizer, such as glycerol or sorbitol. The push-fit capsules can contain the active ingredients in admixture with filler such as lactose, binders such as starches and/or lubricants such as talc or magnesium stearate and, optionally, stabilizers. In soft capsules, the active compounds may be dissolved or suspended in suitable liquids, such as fatty oils, liquid paraffin, or liquid polyethylene glycols. In addition, stabilizers may be added.

A "patient" for the purposes of the present invention, i. e. to whom a compound according to the present invention or a pharmaceutical composition according to the present invention is administered, includes both humans and other animals and organisms. Thus the compounds, pharmaceutical compositions and methods are applicable to or in connection with both human therapy and veterinary applications including diagnostic(s), diagnostic procedures and methods as well as staging procedures and methods. For example, the veterinary applications include, but are not limited to, canine, bovine, feline, porcine, caprine, equine, and ovine animals, as well as other domesticated animals including reptiles, such as iguanas, turtles and snakes, birds such as finches and members of the parrot family, lagomorphs such as rabbits, rodents such as rats, mice, guinea pigs and hamsters, amphibians, fish, and arthropods. Valuable non-domesticated animals, such as zoo animals, may also be treated. In the preferred embodiment the patient is a mammal, and in the most preferred embodiment the patient is human.

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The pharmaceutical composition according to the present invention comprises at least one compound according to the present invention in a form suitable for administration to a patient. Preferably, a compound according to the present application is in a water soluble form, such as being present as a pharmaceutically acceptable salt, which is meant to include both acid and base addition salts which are also generally referred to herein as pharmaceutically acceptable salts. "Acid addition salt", and more particularly "pharmaceutically acceptable acid addition salts" refers to those salts that retain the biological effectiveness of the free bases and that are not biologically or otherwise undesirable, formed with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid and the like, and organic acids such as acetic acid, propionic acid, glycolic acid, pyruvic acid, oxalic acid, maleic acid, malonic acid, succinic acid, fumaric acid, tartaric acid, citric acid, benzoic acid, cinnamic acid, mandelic acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like. "Base addition salts" and more particularly "pharmaceutically acceptable base addition salts" include those derived from inorganic bases such as sodium, potassium, lithium, ammonium, calcium, magnesium, iron, zinc, copper, manganese, aluminum salts and the like. Particularly preferred are the ammonium, potassium, sodium, calcium, and magnesium salts. Salts derived from pharmaceutically acceptable organic nontoxic bases include salts of primary, secondary, and tertiary amines, substituted amines including naturally occurring substituted amines, cyclic amines and basic ion exchange resins, such as isopropylamine, trimethylamine, diethylamine, triethylamine, tripropylamine, and ethanolamine. The pharmaceutical compositions according to the present invention may also include one or more of the following: carrier proteins such as serum albumin; buffers; fillers such as microcrystalline cellulose, lactose, corn and other starches; binding agents; sweeteners and other flavoring agents; coloring agents; and polyethylene glycol. Additives are well known in the art, and are used in a variety of formulations.

The compounds according to the present invention are, in a further embodiment, administered to a subject either alone or in a pharmaceutical composition where the compound(s) is mixed with suitable carriers or excipient(s). In treating a subject, a therapeutically effective dose of compound (i.e. active ingredient) is administered. A therapeutically effective dose refers to that amount of the active ingredient that produces amelioration of symptoms or a prolongation

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of survival of a subject which can be determined by the one skilled in the art doing routine testing.

On the other hand, the compounds according to the present invention may as such or contained in a pharmaceutical composition according to the present invention be used in drug potential applications.

For example, therapeutic agents such as antibiotics or antitumor drugs can be inactivated through the catalytic action of endogenous enzymes, thus rendering the administered drug less effective or inactive. Accordingly, the compound(s) according to the present invention may be administered to a patient in conjunction with a therapeutic agent in order to potentiate or increase the activity of the drug. This co-administration may be by simultaneous administration, such as a mixture of the compound(s) according to the present invention and the drug, or by separate simultaneous or sequential administration.

According to the present invention the compounds disclosed herein, referred to as compounds according to the present invention, may be used as a medicament or for the manufacture of medicament or in a method of treatment of a patient in need thereof. Insofar any of these compounds constitute a pharmaceutical compound. The use of this kind of compound also comprises the use of pharmaceutically acceptable derivatives of such compounds.

In addition, the compounds according to the present invention may be transformed upon application to an organism such as a patient, into the pharmaceutically active compound. Insofar the compounds according to the present invention may be prodrugs which, however, are nevertheless used for the manufacture of the medicaments as disclosed herein given the fact that at least in the organism they are changed in a form which allows the desired.

It is to be understood that any of the pharmaceutical compositions according to the present invention may be used for any of the diseases described herein.

The pharmaceutical compositions according to the present invention may be manufactured in a manner that is known as such, e.g., by means of conventional mixing, dissolving,

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granulating, dragee-mixing, levigating, emulsifying, encapsulating, entrapping, lyophilizing, processes, or the like.

In a further aspect of the present invention the compounds of the present invention may be used as insecticides as they may prevent cell cycle mitosis in insect cells and thus can be used to control the growth and proliferation of a variety of insect pests. This aspect of the present invention has important applications in agriculture, such as in the field, in the storage of agricultural products and the like. Additionally, the compounds according to the present invention are useful for controlling insect populations, preferably in places inhabited by men, such as homes, offices and the like.

Any of the compounds according to the present invention containing one or more asymmetric carbon atoms may occur as racemates and racemic mixtures, single enantiomers, diastereomeric mixtures and individual diastereomers. All such isomeric forms of these compounds are expressly included in the present invention. Each stereogenic carbon may be in the R or S configuration, or a combination of configurations.

It shall be understood by the one of ordinary skill in the art that all compounds of the invention are preferably those which are chemically stable. This applies to any of the various uses of the compounds according to the present invention disclosed herein.

In determining the suitability of any of the compounds according to the present applications for the various uses, besides the particular use-specific profile to be met by such a compound, also it has to be checked whether it is stable to proteolytic degradation. The resistance of the compound used as a pharmaceutical may be tested against a variety of non-commercially available proteases *in vitro* to determine its proteolytic stability. Promising candidates may then be routinely screened in animal models, for example using labelled inhibitors, to determine the *in vivo* stability and efficacy. In any of the aforementioned uses the compound may be present in a crude or purified form. Methods for purifying the compounds according to the present invention are known to the one skilled in the art.

The problem underlying the present invention is also solved by the technical teaching according to the attached independent claims. Preferred embodiments thereof may be taken from the dependent claims.

The invention is now further illustrated by reference to the following figures and examples from which further advantages, features and embodiments may be taken. It is understood that these examples are given for purpose of illustration only and not for purpose of limitation. All references cited herein are incorporated by reference.

- Fig. 1 shows FACS results of compound 703,
- Fig. 2 show a FACS analysis of the effect of various compounds on HL 60 cells as a measure for the apoptotic activity of the compounds; and
- Fig. 3 shows fluorescence microscope photographs of DAPI stained HeLa cells after treatment with various compounds

# Example 1: Material and Methods

In order that the invention herein described may be more fully understood, the following detailed description is set forth. As used herein, the following abbreviations are used:

Ar is argon;

D is doublet;

DCM is dichloromethane;

DIPEA is N,N-diisopropylethylamine;

DMF is N,N-dimethylformamide;

DMSO is N,N-dimethylsulfoxide;

eq is equivalent;

Et₃N is triethylamine;

HCl is chlorhydric acid;

HPLC is high performance liquid chromatography;

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h is hour;
Hz is hertz;
m is multiplet;
mL is milliliter;
NaHCO₃ is sodium hydrogencarbonate;
s is singulet;
THF is tetrahydrofuran.

## Method A: Urea formation in solution

Amine salt and DIPEA (1 eq each) or amine (1 eq) was dissolved in dry dioxan and a solution of the isocyanate (1 eq) in DCM or DMSO was added under Ar in one portion. The solution was stirred for 3 h at room temperature. The solution was diluted with 2 ml DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added to remove unreacted isocyanate, amine and electrophilic impurities respectively. After 18 h at 40°C, the solution was filtered off and the solvent was removed under reduced pressure. The obtained crude ureas were purified by HPLC.

# Method B: Coupling of substituted anilines with sulfonyl chlorides

Aniline (30 mg) and NEt₃ (1.2 eq, 2.2 eq. when HCl salt) were dissolved in dry acetonitrile (0.5 mL). Sulfonyl chloride (1 eq) was dissolved in dry acetonitrile (0.5 mL) and added to the solution. The reaction mixture was stirred under argon for 12 h at 40°C. Tris-(2-aminoethyl)-amine polystyrene (30 mg), (polystyrylmethyl) trimethylammonium bicarbonate (30 mg), N-(2-mercaptoethyl)amino methyl polystyrene (30 mg), and methylisocyanate polystyrene (30 mg) were given to the solution and stirred for additional 12 h at 40°C. After filtration the solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase.

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## Method C: Coupling of substituted anilines with acid chlorides

Aniline (30 mg) and NEt₃ (1 eq, 2 eq. when HCl salt) were dissolved at 0°C in dry DCM (0.5 mL) with 10% DMSO. Acid chloride (1 eq) was dissolved at 0°C in dry DCM (0.5 mL) and added to the solution. The reaction mixture was stirred under argon for 2 h while slowly warming up to room temperature. Work up was performed by pouring the reaction mixture with DCM over incubated HYDROMATRIX layers. 2 mL basic layer (saturated NaHCO₃ solution 2 ml/g HYDROMATRIX), 2 mL acidic layer (2M HCl 2 ml/g HYDROMATRIX), and 2 mL of dry HYDROMATRIX layer in a 10 ml syringe were used. The solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase.

## Method D: Reductive amination of aldehydes with hydroxyl anilines

Amine hydrochloride (0.11 mmol, 1 eq), aldehyde (0.11 mmol, 1 eq), and DIPEA (0.11 mmol, 1 eq) were dissolved in anhydrous THF (1 mL), and molecular sieves 4Å (10 mg) was for 1.5 h at room temperature, After shaking solution. the added to (polystyrylmethyl)trimethylammonium cyanoborohydride (4.3 mmol/g, 0.22 mmol) was added to the reaction mixture. After shaking for 8 h at room temperature, 4-(3 mmol/g, 0.22 mmol), 3-(4polystyrene benzyloxybenzaldehyde (hydrazinosufonyl)phenyl)propionyl AM resin (1.5 mmol/g, 0.22 mmol), and N-(2mercaptoethyl)aminomethyl polystyrene (2.1 mmol/g, 0.22 mmol) were added, after which the reaction mixture was shaken at room temperature for 18 h. Filtration, washing with DCM, and evaporation of the solvent in vacuo afforded the crude product, which was purified by reversed phase HPLC.

# Method E: Condensation of amines with hydroxyl carboxylic acids

1-Ethyl-3(3'-dimethylaminophropyl)carbodiimide hydrochloride (0.15 mmol, 1.36 eq), hydroxyl carboxylic acid (0.15 mmol, 1.36 eq), and 1-hydroxy-7-azabenzotriazole (0.15 mmol, 1.36 eq) were dissolved in DMF (0.7 mL). After shaking for 30 min at room temperature, a solution of amine (0.11 mmol) in DMF (0.7 mL) was added to the reaction mixture. After shaking for 2 h at room temperature, amine (0.22 mmol) was added, after which the reaction mixture was shaken at 60 °C overnight. Then the solvent was evaporated in vacuo, and the residue was dissolved in DCM (7 mL). HYDROMATRIX™ (0.3 g) which

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was previously treated with HCl (2N, 0.6 mL) was added to the solution, and the mixture was shaken for 30 min. Filtration, washing with DCM, and evaporation of the solvent in vacuo afforded the crude product, which was purified by reversed phase HPLC.

#### Method F: Carbamate formation in solution

Amine or amine salt (1 eq) and sodium bicarbonate (1 or 2 eq) were dissolved in a mixture of MeOH / H₂O (3:1). The mixture was treated with chloroformate (1 eq), which was added in three portions over 10 minutes. After 30 minutes at room temperature, the precipitating product was collected by filtration and washed with water. The obtained crude carbamates were purified by HPLC.

## Method G: Carbamate formation in solution

To an ice cooled mixture of amine or amine salt (1 eq) and DIPEA (1.1 eq or 2.2 eq) in dry DCM was added an ice cooled solution of chloroformate (1.1 eq) in DCM in one portion. After 1.5-8 h at room temperature the solvent was removed under reduced pressure. The obtained crude carbamates were purified by HPLC.

#### Method H: Carbamate formation in solution

To a mixture of amine or amine salt (1 eq) and sodium bicarbonate (1 or 2.5 eq) in dry DCM was added chloroformate (1 eq) in one portion. After 4 hours at room temperature the sodium bicarbonate was filtered off and the solvent was removed under reduced pressure. The obtained crude carbamates were purified by HPLC.

#### Method I: Thiourea formation in solution

Amine salt and DIPEA (1 eq each) or amine (1 eq) was dissolved in dry dioxan and a solution of the thioisocyanate (1 eq) in DCM or DMSO was added under Ar in one portion. The solution was stirred for 3 h at room temperature. The solution was diluted with 2 ml DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added to remove

unreacted isocyanate, amine and electrophilic impurities respectively. After 18 h at 40°C, the solution was filtered off and the solvent was removed under reduced pressure. The obtained crude thioureas were purified by HPLC.

## Method J: Synthesis of (3-amino-5-chloro-4-hydroxy-phenyl)-ureas.

Isocyanate (5.0 mmol) was added to a stirred solution of 4-Amino-2-chloro-phenol (5.0 mmol) in anhydrous CH₂Cl₂ (23 mL) and THF (4 mL) at room temperature. After stirring for 12 h, the solvent was evaporated in vacuo. The residue was then dissolved in HOAc (95 mL) and added in one single portion to a stirred solution of NaNO₂ (1.17 g, 17.0 mmol) in H₂O (8.4 mL). The flask was sealed with a stopper and the reaction mixture was stirred for 1.5 min at room temperature. The reaction was stopped by the addition of saturated aqueous NaHCO₃ (190 mL). After stirring for 10 min at room temperature, the yellow precipitate was filtered, washed with H₂O (3 x 30 mL), and dried in vacuo. The yellow residue was then dissolved in a mixture of toluene (75 mL) and MeOH (90 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 2 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding diureas by method A, the corresponding amilines by method C or E, or the corresponding thioureas by method I.

Method K: Synthesis of (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-ureas, (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-thioureas, (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-ureas, (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-thioureas, (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-amides, and (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-amides.

3-Chloro-2-hydroxy-5-nitro-benzoic acid or 3-chloro-4-hydroxy-5-nitro-benzoic acid (0.41 g, 1.9 mmol) was dissolved in polyphosphoric acid (12.3 g) at 110 °C. 2-Aminothiophenol (0.36 mg, 2.9 mmol) was added and the resulting solution was stirred at 110 °C for 5 h. After cooling, ammonia (35% in  $H_2O$ , 12 mL) was added to the reaction mixture. The precipitate was filtered, washed with  $H_2O$  (3 x 10 mL) and dried in vacuo. The residue was then

dissolved in a mixture of MeOH (30 mL) and THF (70 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 1 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding ureas by method A, the corresponding amides by method C or E, or the corresponding thioureas by method I.

# Method L: Synthesis of (3-amino-5-chloro-4-hydroxy-phenyl)-amides.

Acyl chloride (5.0 mmol) was added to a stirred solution of 4-Amino-2-chloro-phenol (5.0 mmol) in anhydrous CH₂Cl₂ (23 mL) and THF (4 mL) at O°C. After stirring for 12 h, the solvent was evaporated in vacuo. The residue was then dissolved in HOAc (95 mL) and added in one single portion to a stirred solution of NaNO₂ (1.17 g, 17.0 mmol) in H₂O (8.4 mL). The flask was sealed with a stopper and the reaction mixture was stirred for 1.5 min at room temperature. The reaction was stopped by the addition of saturated aqueous NaHCO₃ (190 mL). After stirring for 10 min at room temperature, the yellow precipitate was filtered, washed with H₂O (3 x 30 mL), and dried in vacuo. The yellow residue was then dissolved in a mixture of toluene (75 mL) and MeOH (90 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 2 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding ureas by method A, the corresponding anilines by method C or E, or the corresponding thioureas by method I.

Example 2: 1-Adamantan-1-yl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-urea

To a solution of 6-amino-2,4-dichloro-3-methyl-phenol hydrochloride (113.5 mg, 1 eq) and DIPEA (48 μL, 1 eq) in dioxan (1.1 mL) was added 1-adamantylisocyanate (88.5 mg, 1 eq) in 580 μL DMSO in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 40°C the solution was filtered off and the solvent was removed under reduced pressure. The crude product was purified by HPLC to obtain 118 mg (64 %) of the title compound as a white powder.

NMR-¹H (DMSO-d₆)  $\delta = 1.62$  (s_b, 6H), 1.92 (s_b, 6H), 2.05 (s_b, 3H), 2.29 (s, 3H), 6.79 (s, 1H), 7.95 (s, 1H), 8.15 (s, 1H), 9.82 (s, 1H).

NMR- 13 C (DMSO- 13 C (DMSO-

Example 3: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea

To a solution of 4-amino-2,6-dichloro-phenol (44.5 mg, 1 eq) in dioxan (2.0 mL) was added 2-isocyanato-2,4,4-trimethyl-pentane (38 mg, 1 eq) in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 35°C the solution was filtered off and the solvent was removed under reduced pressure. The crude material was purified by HPLC to obtain 67 mg (81%) of the title compound as a white powder.

NMR-¹H (DMSO-d₆)  $\delta$  = 0.95 (s, 9H), 1.30 (s, 6H), 1.70 (s, 2H), 2.30 (s, 3H), 6.80 (s, 1H), 8.00 (s, 1H), 8.08 (s, 1H), 9.83 (s_b, 1H).

NMR-¹³C (DMSO-d₆)  $\delta$  = 29.7, 31.2, 50.5, 53.2, 117.3, 122.4, 134.0, 142.8, 153.9; MS (m/z): 333.2 [M+H⁺].

Example 4: 2 N-(2-Hydroxy-4-methyl-phenyl)-C-phenyl-methanesulfonamide

The compound was obtained in 32% yield (21.2 mg) using the protocol described in method A.

NMR-¹H (DMSO-d₆)  $\delta$  = 2.13 (s, 3H), 4.97 (s, 2H), 6.70 (d, 1H, J = 8.2 Hz), 6.78 (s, 1H), 6.83 (d, 1H, J = 8.2 Hz), 7.43 (m, 2H), 7.49 (m, 2H); MS (m/z): 278.1 [M⁺].

Example 5: Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide

The compound was obtained in 47% yield (22.1 mg) using the protocol described in method B.

NMR-¹H (DMSO-d₆)  $\delta = 2.25$  (d, 6H, J = 6.8), 2.27 (s, 3H), 3.97 (hep, 1H, J = 6.8), 5.39 (s, 1H), 6.91 (s, 1H); MS (m/z): 298.1 [MH⁺].

Example 6: N-(3,5-Dichloro-2-hydroxy-phenyl)-2-phenyl-acetamide

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The compound was obtained in 22% yield (11.0 mg) using the protocol described in method C.

NMR-¹H (DMSO-d₆)  $\delta$  = 3.06 (s, 2H), 7.25 (m, 1H), 7.31 (m, 2H), 7.32 (m, 2H), 7.61 (m, 2H), 9.87 (m, 1H); MS (m/z): 296.2 [MH⁺].

Example 7: N-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-N-methyl-2-trifluoromethyl-benzamide

Aniline HCL salt (300 mg, 1.3 mmol) and K₂CO₃ (500 mg) were dissolved in DMSO (5 mL). CH₃I (187 mg, 1.3 mmol) was added and the suspension was stirred for 48 h at room temperature. After filtration, the solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase to give the *N*-methyl amino phenol derivative (130 mg, 31 %).

The amide was obtained in 56% yield (19.7 mg) using the protocol described in method C. NMR- 1 H (DMSO-d₆)  $\delta$  = 2.41 (s, 3H), 3.75 (s, 3H), 7.70–7.85 (m, 4H), 8.05 (d, 1H, J = 5.0); MS (m/z): 377.9 [MH $^{+}$ ].

Example 8: 2,4-Dichloro-3-methyl-6-(3-methyl-benzylamino)-phenol

The compound was obtained in 49 % yield (16 mg) using the protocol described in method D. According to method D.

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NMR- 1 H (DMSO- 1 d₆)  $\delta$  2.21 (s, 3 H), 2.27 (s, 3 H), 4.27 (s, 2 H), 5.80 (br s, 1 H), 6.35 (s, 1 H), 7.02-7.24 (m, 4 H), 9.18 (br s, 1 H); MS (m/z): 296.2 [M+H $^{+}$ ].

Example 9: 1-{5-Chloro-3-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone

The compound was obtained in 18 % yield (12 mg) using the protocol described in method D. NMR- 1 H (DMSO-d₆)  $\delta$  2.60 (s, 3 H), 4.40 (s, 2 H), 6.24 (d, J = 2.0 Hz, 1H), 6.41 (m, 1H), 7.10 (d, J = 2 Hz, 1H), 7.18-7.24 (m, 2 H), 7.29-7.44 (m, 6 H), 12.66 (s, 1 H); MS: m/z: 418.5 [M+H⁺].

Example 10: 4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol

The compound was obtained in 34 % yield (23 mg) using the protocol described in method D. NMR- 1 H (DMSO- 1 d₆)  $\delta$  1.27 (d, J = 6.4 Hz, 3 H), 4.33 (s, 2 H), 4.97 (q, J = 6.4 Hz, 1 H), 5.96 (d, J = 2.4 Hz, 1 H), 6.47 (d, J = 2.4 Hz, 1 H), 7.19-7.47 (m, 8 H), 8.69 (br. S, 1 H); MS: m/z: 420.7 [M+H⁺].

Example 11: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 26 % yield (11 mg) using the protocol described in method F. NMR-¹H (DMSO-d₆)  $\delta$ = 7.25 (m, 3H), 7.43 (m, 2 H), 7.50 (s, 2H) NMR- 13 C (DMSO- 13 C)  $\delta = 109.1$ , 118.8, 121.4, 128.2, 129.4, 132.6, 153.2, 157.3

Example 12: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid phenyl ester

The compound was obtained in 31 % yield (24 mg) using the protocol described in method F. NMR- 1 H (DMSO- 1 d₆)  $\delta$  = 2.38 (s, 3 H), 6.76 (m, 3H), 7.15 (m, 3H) NMR- 13 C (DMSO-d₆)  $\delta$ = 16.5, 109.1, 115.2, 118.8, 126.7, 128.5, 129.5, 129.7, 139.4, 153.4, 157.4

Example 13: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid benzyl ester

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According to method F 2-amino-4,6-dichloro-phenol (25 mg, 1 eq) and phenylchloroformate (23  $\mu$ L, 1 eq) gave 10.9 mg (26 %) of the title compound as a white solid. NMR-¹H (DMSO-d₆)  $\delta$ = 5.30 (d, 2 H), 7.43 (m, 2 H), 7.25 (m, 2H), 7.50 (s, 2H)

Example 14: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

The compound was obtained in 39% yield (22 mg) using the protocol described in method G. NMR- 1 H (DMSO- 1 d₆)  $\delta$  = 0.84-0.90 (m, 3H), 1.22-1.41 (m, 6H), 2.35 (s, 3H), 3.28-3.33 (m, 2H), 4.06 (t, 2H), 7.57 (s, 1H), 8.74 (s, 1H).

Example 15: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

The compound was obtained in 54% yield (44 mg) using the protocol described in method G. NMR- 1 H (DMSO- 1 d₆)  $\delta$  = 0.75 (d, 3H), 0.82-093 (m, 7H), 0.96-1.14 (m, 2H), 1.29-1.53 (m, 2H), 1.59-1.71 (m, 2H), 1.88-2.02 (m, 2H), 4.54 (ddd, 1H), 7.47 (s, 2H), 9.67 (s, 1H), 9.73 (s, 1H)

Example 16: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid hexyl ester

The compound was obtained in 21% yield (10 mg) using the protocol described in method G. NMR- 1 H (DMSO- 1 d₆)  $\delta$  = 0.87 (t, 3H), 1.25-1.40 (m, 6H), 1.55-1.66 (m, 2H), 2.35 (s, 3H), 4.06 (t, 2H), 7.56 (s, 1H), 8.74 (s, 1H), 9.73 (s, 1H).

Example 17: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid hexyl ester

The compound was obtained in 43% yield (30 mg) using the protocol described in method G. NMR- 1 H (DMSO-d₆)  $\delta$  = 0.87 (t, 3H), 1.21-1.40 (m, 6H), 1.54-1.66 (m, 2H), 4.06 (t, 2H), 7.46 (s, 2H), 9.67 (s, 1H), 9.73 (s, 1H).

Example 18: 1-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea

The compound was obtained in 31% yield (16 mg) using the protocol described in method J. NMR- 1 H (DMSO- 1 d₆)  $\delta$  1.06 (s, 9 H), 1.08-1.28 (m, 5 H), 1.35 (s, 6 H), 1.45-1.76 (m, 7 H), 3.30-3.42 (m, 1 H), 6.84 (s, 1 H), 7.24 (s, 1 H), 7.73 (s, 1 H), 8.20 (br. s, 1 H), 8.82 (s, 1 H), 8.97 (s, 1 H), 9.11 (s, 1 H); MS: m/z: 439.2 [M+H⁺].

Example 19: N-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-2-nitrobenzenesulfonamide

According to method J 1-(3-amino-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (19 mg, 67 μmol) and 2-nitro-benzenesulfonyl chloride (15 mg, 67 μmol) gave N-[3-Chloro-5-(3cyclohexyl-ureido)-2-hydroxy-phenyl]-2-nitro-benzenesulfonamide (15 mg, 48%). NMR- 1 H (DMSO- 1 d₆)  $\delta$  1.05-1.37 (m, 5 H), 1.49-1.83 (m, 5 H), 3.42-3.47 (m, 1 H), 5.94 (d, J= 7.9 Hz, 1 H), 6.99 (d, J = 2.4 Hz, 1 H), 7.46 (d, J = 2.4 Hz, 1 H), 7.78-7.90 (m 2 H), 7.93-7.908.03 (m, 2 H), 8.27 (s, 1 H), 9.19 (br s, 1 H), 9.70 (s, 1 H); MS: m/z: 469.1 [M+H⁺].

Example 20: 1-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea

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According to method K 4-amino-2-benzothiazol-2-yl-6-chloro-phenol (21 mg, 76 µmol) and isocyanato-cyclohexane (9.5 mg, 76 µmol) gave 1-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (3.0 mg, 10%).

NMR-¹H (DMSO-d₆)  $\delta$  1.09-1.41 (m, 5 H), 1.49-1.87 (m, 5 H), 3.41-3.47 (m, 1H), 6.12 (d, J = 7.8 Hz, 1 H), 7.51 (t, J = 7.8 Hz, 1 H), 7.60 (t, J = 7.1 Hz, 1 H), 7.68 (d, J = 2.4 Hz, 1 H), 8.06 (d, J = 2.4 Hz, 1 H), 8.11 (d, J = 8.3 Hz, 1 H), 8.21 (d, J = 7.3 Hz, 1 H), 8.52 (s, 1 H), 11.92 (s, 1 H); MS: m/z: 402.2 [M+H⁺].

Example 21: 1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-(2-trifluoromethyl-phenyl)-thiourea

According to method K 2-Amino-4-benzothiazol-2-yl-6-chloro-phenol (20 mg, 72 μmol) and 1-isothiocyanato-2-trifluoromethyl-benzene (15 mg, 72 μmol) gave 1-(5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-(2-trifluoromethyl-phenyl)-thiourea (12 mg, 35%).

NMR- 1 H (DMSO- 1 d₆)  $\delta$  7.40-7.56 (m, 3 H), 7.66-7.79 (m, 3 H), 7.92 (d, J = 2.4 Hz, 1 H), 8.03 (d, J = 7.8 Hz, 1 H), 8.12 (d, J = 8.8 Hz, 1 H), 8.68 (br s, 1 H), 9.65 (s, 1 H), 9.94 (s, 1 H), 10.65 (s, 1 H); MS: m/z: 480.0 [M+H⁺].

Example 22: 1-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-3-(4-trifluoromethyl-phenyl)-thiourea

The compound was obtained in 57% yield (59 mg) using the protocol described in method I. NMR- 1 H (DMSO- 1 d₆)  $\delta = 2.38$  (s, 3 H), 7.68-7.85 (m, 5 H), 9.43 (s, 1 H), 9.90 (s, 1 H), 10.37 (s, 1 H); MS (m/z): 278.1 [M⁺].

Example 23: 1-Adamantan-1-yl-3-(3,5-dichloro-4-hydroxy-phenyl)-urea

The compound was obtained in 60% yield (35 mg) using the protocol described in method A. NMR- 1 H (DMSO- 1 d₆)  $\delta = 1.60$  (s_b, 6H), 1.95 (s_b, 6H), 2.08 (s_b, 3H), 6.79 (s, 1H), 7.95 (s, 1H), 8.18 (s, 1H), 9.82 (s, 1H).

NMR- 13 C (DMSO- 13 C (DMSO- 13 C)  $\delta = 17.2, 29.5, 36.1, 41.7, 50.3, 116.2, 122.2, 123.8, 124.8, 140.6, 154.3; MS (m/z): 369.2 [M+H⁺].$ 

Example 24: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea

To a solution of 4-amino-2,6-dichloro-phenol (44.5 mg, 1 eq) in dioxan (2.0 mL) was added 2-isocyanato-2,4,4-trimethyl-pentane (38 mg, 1 eq) in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 35°C the solution was filtered off and the solvent was removed under reduced pressure. The crude material was purified by HPLC to obtain 67 mg (81%) of the title compound as a white powder.

NMR-¹H (DMSO-d₆)  $\delta$  = 0.95 (s, 9H), 1.28 (s, 6H), 1.69 (s, 2H), 5.90 (s, 1H), 7.33 (s, 2H), 8.22 (s, 1H), 9.50 (s_b, 1H).

NMR-¹³C (DMSO-d₆)  $\delta$  = 29.9, 31.2, 50.9, 54.2, 117.3, 121.4, 134.0, 142.8, 152.9; MS (m/z): 333.2 [M+H⁺].

Example 25: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-thiourea

The compound was obtained in 58% yield (34.8 mg) using the protocol described in method I. NMR- 1 H (DMSO- 1 G)  $\delta = 6.32$  (m, 2 H), 6.80 (m, 2 H), 7.42 (m, 2 H), MS (m/z): 381.2 [M $^{+}$ ].

Example 26: Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide

The compound was obtained in 40% yield (21 mg) using the protocol described in method B.

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NMR-¹H (DMSO-d₆)  $\delta = 2.43$  (d, 6H), 2.51 (s, 3H), 3.97 (m, 1H), 5.43 (s, 1H), 6.8 (s, 1H); MS (m/z): 284.1 [MH⁺].

Example 27: N-(3,5-Dichloro-4-hydroxy-phenyl)-2-phenyl-acetamide

The compound was obtained in 22% yield (11.0 mg) using the protocol described in method C.

NMR-¹H (DMSO-d₆)  $\delta$  = 3.12 (s, 2H), 7.24 (m, 1H), 7.36 (m, 2H), 7.37 (m, 2H), 7.61 (m, 2H), 9.91 (m, 1H); MS (m/z): 296.2 [MH⁺].

Example 28: 2,6-Dichloro-4-(3-methyl-benzylamino)-phenol

The compound was obtained in 55% yield (15.0 mg) using the protocol described in method D.

NMR- 1 H (DMSO-d₆)  $\delta$  2.26 (s, 3 H), 4.29 (s, 2 H), 5.92 (s, 1 H), 6.50 (s, 1 H), 7.00-7.28 (m, 4 H), 9.20 (s, 1 H); MS (m/z): 282.2 [M+H $^{+}$ ].

Example 29: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 49% yield (55.7 mg) using the protocol described in method F.

NMR-¹H (DMSO-d₆)  $\delta$  = 7.22 (m, 2H), 7.36 (m, 2 H), 7.50 (s, 2H) NMR-¹³C (DMSO-d₆)  $\delta$  = 118.5, 121.9, 122.5, 125.5, 129.4, 131.7, 144.7, 150.3, 151.6

Example 30: (3-Chloro-4-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 46% yield (32.1 mg) using the protocol described in method F.

NMR-¹H (DMSO-d₆)  $\delta$  = 2.38 (s, 3 H), 6.76 (s, 1H), 7.15 (m, 5H), 7.32 (m, 2 H). NMR-¹³C (DMSO-d₆)  $\delta$  = 16.5, 109.1, 115.2, 118.8, 126.7, 128.5, 129.5, 129.7, 139.4, 153.4, 157.4

Example 31: (3,5-Dibromo-4-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 25 % yield (10.2 mg) using the protocol described in method F.

NMR-¹H (DMSO-d₆)  $\delta$  = 7.33 (m, 2 H), 7.45 (m, 2H), 7.50 (s, 2H)

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Example 32: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

According to method G 4-amino-2,6-dichloro-phenol (40 mg, 1 eq) and (-)-menthylchloroformate (54  $\mu$ l, 1.1 eq) in DCM gave 44.1 mg (54 %) of the title compound as a white solid.

NMR-¹H (DMSO-d₆)  $\delta$  = 0.71 (d, 3H), 0.78-0.96 (m, 7H), 0.99-1.16 (m, 2H), 1.29-1.58(m, 2H), 1.59-1.71 (m, 2H), 2.0-2.15 (m, 2H), 4.58 (m, 1H), 7.49 (s, 2H), 9.68 (s, 1H), 9.73 (s, 1H)

Example 33: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid hexyl ester

According to method G 4-amino-2,6-dichloro-phenol (40 mg, 1 eq) and hexylchloroformate (41  $\mu$ L, 1.1 eq) gave 30 mg (43 %) of the title compound as a white solid.

NMR-¹H (DMSO-d₆)  $\delta$  = 0.75 (m, 3H), 1.21-1.40 (m, 6H), 1.48-1.62 (m, 2H), 4.22 (m, 2H), 7.32 (s, 2H), 9.69 (s, 1H), 9.75 (s, 1H).

Example 34: 1-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(2-trifluoromethylphenyl)-urea

According to method J 1-(3-amino-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (30 mg, 0.11 mmol) and 1-isocyanato-2-trifluoromethyl-benzene (21 mg, 0.11 mmol) gave 1-[3chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(2-trifluoromethyl-phenyl)-urea (16 mg, 31%).

NMR- 1 H (DMSO- 1 d₆)  $\delta$  0.98-1.28 (m, 5 H), 1.39-1.76 (m, 5 H), 3.30-3.42 (m, 1 H), 5.84 (d, J = 7.8 Hz, 1 H), 7.24 (d, J = 7.8 Hz, 1 H), 7.31 (d, J = 2.4 Hz, 1 H), 7.52-7.67 (m, 2 H), 7.71-7.75 (m, 2 H), 8.20 (br. s, 1 H), 8.80-8.82 (m, 1 H), 8.97-9.04 (m, 1 H), 9.11 (s, 1 H); MS: m/z: 471.1 [M+H⁺].

# Example 35: Specificity of inhibition of certain enzymes by compounds according to the present invention

In order to characterize the specificity of various compounds the following assays were performed. PPIase activity of hPin1, hCyp18, LpCyp18, hFKBP12 and EcParvulin was measured using the protease-coupled PPIase assay according to Fischer et al. (Fischer, G.; Bang, H.; Mech, C. Determination of enzymatic catalysis fort he cis-trans-isomerization of peptide binding in proline-containing peptides. [German] Biomed. Biochem. Acta 1984, 43, 1101-1111; Hennig et al., Selective Inactivation of Parvulin-like peptidyl-prolyl cis/trans isomerases by Juglon, Biochemistry. 1998, 37(17):5953-5960). For hPin1 measurements Ac-Ala-Ala-Ser(PO3H2) -Pro-Arg-pNA was used as a substrate and trypsin (final concentration

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190 μg/ml) as an isomer-specific protease. Activity measurements of other PPIases were made with the substrate peptide Suc-Ala-Phe-Pro-Phe-pNA and the protease -chymotrypsin (final concentration 470 μg/ml). The assays were performed in a final reaction volume of 150 μl at final concentrations of 6 nM hPin1, 10 nM hCyp18, 5 nM LpCyp18, 20 nM EcParvulin and 20 nM hFKBP12, respectively, and 120 μM substrate peptide in 35 mM HEPES (pH 7.8). For inhibition experiments 100-0.01 μM of effector freshly diluted from a DMSO stock solution were added. The amount of solvent was kept constant within each experiment, usually below 0.3% (v/v). All reactions were started by addition of protease. The test was performed by observing the released 4-nitroaniline at 390 nm with a MR5000 UV/Vis spectrophotometer (Dynex) at 6°C. Data were evaluated by calculation of pseudo-first-order rate constants k_{obs} in presence of PPIase and PPIase/effector, respectively, and corrected for the contribution of the non-catalyzed reaction (k₀). Inhibition constants IC₅₀ were calculated using SigmaPlot 8.0 (SPSS).

The following target enzymes which are all rotamases belonging to different classes of rotamases were used:

- T-1: Protein interacting with NIMA (-kinase), hPin1
- T-2: First described human Rapamycin receptor, hFKBP12
- T-3: Human Cyclosporin A receptor with 18 kDa molecular weight, hCyp18
- T-4: Leishmonia pneumophila virulence Cyclosporin A receptor with 18 kDa molecular weight, LpCyp18
- T-5: Bacterial Juglon sensitive non proteolytic enzyme, EcParv

These rotamases are known in the art. Their production and characteristics may be taken from the following references.

#### Review about all PPIase families

Gothel, S. F.; Marahiel, M. A. TI Peptidyl-prolyl cis-trans isomerases, a superfamily of ubiquitous folding catalysts [Review]. Cell. Molec. Life Sci. 1999, 55, 423-436

#### Pin1

Lu, K. P.; Hanes, S. D.; Hunter, T. (1996) A human peptidyl-prolyl isomerase essential for regulation of mitosis. *Nature* 1996, 380, 544-547

Yaffe, M. B.; Schutkowski, M.; Shen, M. H.; Zhou, X. Z.; Stukenberg, P. T.; Rahfeld, J. U.; Xu, J.; Kuang, J.; Kirschner, M. W.; Fischer, G.; Cantley, L. C.; Lu K. P. SEQUENCE-SPECIFIC AND PHOSPHORYLATION-DEPENDENT PROLINE ISOMERIZATION - A POTENTIAL MITOTIC REGULATORY MECHANISM. Science 1997, 278, 1957-1960

Shen, M.; Stukenberg, P. T.; Kirschner, M. W.; Lu, K. P. The essential mitotic peptidyl-prolyl isomerase Pin1 binds and regulates mitosis-specific phosphoproteins. *Genes Developm.* 1998, 12, 706-720.

#### **EcParvulin**

Rahfeld JU. Schierhorn A. Mann K. Fischer G. A novel peptidyl-prolyl cis/trans isomerase from Escherichia coli. FEBS Letters. 1994, 343, 65-69

Rahfeld JU. Rucknagel KP. Schelbert B. Ludwig B. Hacker J. Mann K. Fischer G. Confirmation of the existence of a third family among peptidyl-prolyl cis/trans isomerases. Amino acid sequence and recombinant production of parvulin. *FEBS Letters.* 1994, 352, 180-184

# FKBPs (including FKBP12) and Cyclophilins (including Cyp18)

For recent reviews on cyclophilins and FKBPs and their effectors, see: (a) Fischer, G. Peptidyl-prolyl cis/trans isomerases and their effectors. Angew. Chem., Int. Ed. Engl. 1994, 33, 1415-1436. (b) Galat, A.; Metcalfe, S. M. Peptidylproline cis/trans isomerases. Prog. Biophys. Molec. Biol. 1995, 63, 67-118.

### LpCyp18

Schmidt B. Tradler T. Rahfeld JU. Ludwig B. Jain B. Mann K. Rucknagel KP. Janowski B. Schierhorn A. Kullertz G. Hacker J. Fischer G. A cyclophilin-like peptidyl-prolyl cis/trans

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isomerase from Legionella pneumophila--characterization, molecular cloning and overexpression. *Mol. Microbiol.* 1996, 21,1147-1160

In order to cluster the various rotamase inhibitors the following classes were defined with "A" indicating the most potent rotamase inhibitor.

A: IC50 < 1  $\mu$ M

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \,\mu\text{M} < \text{IC}50 < 50 \,\mu\text{M}$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E:  $IC50 > 100 \mu M$ 

Table 2

Specificity of the inhibition with rotamases

A: IC50 < 1  $\mu$ M

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \mu M < IC50 < 50 \mu M$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E: IC50 > 100  $\mu$ M

Table 2
Specificity of the inhibition with rotamases

	N°		Target				
Compound		T-1	T-2	T-3	T-4	T-5	
CI OH N	120	С	D	С	E	•	

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI CI	655	C	E	Е	E	С
CI CI CI	512	С	E	D	E	С
CI SO2	563	В	В	E ·	Е	E
CI CI	109	A	E	С	E	С
CI OH II	599	В	Е	Е	D	С
CI CI	118	В	D	C	С	В
	643	С	Е	E	Е	E
HO CI	605	A	Е	С	E	В

	N _o			Target		
Compound		T-1	T-2	T-3	T-4	T-5
OH HN S	. <b>26</b> 6	<b>A</b>	E	E	E	В
CI CI	629	A	E	С	E	В
CI CI	102	В	Е	C .	С	В
CI CI	30	В	E	E	Е	E
CI S CF3	264	A	-	-	-	-
OH H H	254	A	_	· <b>-</b>	-	-
CI N S	639	A	<b>-</b>	_	-	-

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI S N	640	В	_	-	-	-
CI SI	257	<b>A</b>	-	-	-	-
F H H H	126	A	-	•	-	-
F N N N	127	В	-	-	-	-
P OH I I	142	A	-	<b>.</b>	-	-
CI CI	31	A	-	1	-	1
CI CI	593	В	-	-	-	-

_	No		<del>- 1</del>	Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI N IN	637	В	-	ı	-	-
CI S N	638	В	-	_	-	-
CI H H H	636	A	-	ı	-	•
CI HN	622	A	-	• <del>-</del>	-	-
CI HN N	656	Α .	-	-	-	-

Company	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI CI CI	.371	A	E	С	E	C
HO CI	672	A	С	В	. <b>C</b>	С
CI OH II	647	В	E	E	E	E
ĕ → C	483	В	Е	С	E	D
CI CI CI	482	В	Е	C	E	E
CI S CI	343	В	E	С	E	Е

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI S CI	441	В	E	С	В	E
F OH S CI	399	A	E	D	D	С
CI HN S CI	610	A	-	-	-	-
CI OH CI OH CI	673	A	-	-	-	-
F NO ₂	400	A	-		-	
CI HO CI	719	A	E	D	С	-
CI CI	703	A	Е	Е	E	В

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
HO CI	.700	A	E	E	Е	С
CI HO CI	710	A	E	Е	E	E
CI CI	716	В	<b>E</b> .	E	E	C
HO CI	1273	A	Е	E	E	В
CI HO CI	1293	В	E	E	E	С
CI NO2	1294	A	E	E	E	В
CI CF3	894	A	E	E	E	В
CI HO CI	1295	В	E	E	E	В

	N°			Target	· · · · · · · · · · · · · · · · · · ·	
Compound		T-1	T-2	T-3	T-4	T-5
HO CI	1296	В	E	C	E	С
CI HO CI	1297	A	E	E	E	C
CI CI	1298	A	E	E	E	С
CI THE STATE OF TH	1299	A	Е	A	E	С
HO CI	1044	A	С	C	В	С

As may be taken from the above table 2 the following compounds 24, 88, 89, 110, 169, 170, 298, 342, 344, 377, 378, 700, 703, 710, 894, 1273, 1294, 1297 are of class A and are thus extremely specific for hPin1.

# Example 36: Specificity of inhibition of proteases

In order to investigate the impact of some of the inventive compounds on the activity of key proteases the following assay was performed: Protease activities were measured

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spectrophotometrically at 30°C according to Schomburg and Salzmann (Schomburg, B.; Salzmann M. GBF: Enzyme Handbook. Springer Verlag, Berlin Heidelberg, 1991) and Bergmeyer et al. (Bergmeyer, H. U.; Bergmeyer, J.; Graßl, M. Methods of Enzymatic Analysis, Vol. V Enzymes 3: Peptides, Proteinases and Their Inhibitors. pp 55 – 371, VCH, Weinheim, 1988). The release of 4-nitroaniline was determined at 390 nm with a Spectramax Plus UV/Vis spectrophotometer (Molecular Devices). The cathepsin B assay was performed in a reaction mixture containing 0.2 μg/ml cathepsin B, 2 mM Z-Arg-Arg-pNA in 88 mM KH₂PO₄, 12 mM Na₂HPO₄, 1.33 mM EDTA, 0.03% Brij 35 (pH 5.8). The trypsin assay was carried out in a reaction mixture containing 0.1 μg/ml trypsin and 120 μM Ac-Ala-Ala-Ser(PO₃H₂) -Pro-Arg-pNA in 35 mM HEPES (pH 7.8) and the papain assay in a mixture consisting of 16 μg/ml papain and 2 mM Bz-DL-Arg-pNA in 10 mM Na₂HPO₄, 2 mM L-Cys, 5 mM EDTA (pH 6.5). In general, reactions were started by addition of peptide substrate after a 30 min incubation of 1-100 μM effector with given concentrations of enzyme.

The key proteases used were the following:

T-6: Papain

T-7: Trypsin

T-8: Cathepsin

In order to cluster the various compounds the following classes of activity were defined.

A:  $IC50 < 1 \mu M$ 

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \mu M < IC50 < 50 \mu M$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E:  $IC50 > 100 \mu M$ 

Table 3
Specificity of the inhibition of some proteases

	No		Target	
Compound		T-6	T-7	T-8

	N°		Target	
Compound		Т-6	T-7	T-8
CI CI	102	D	С	D
CI CI	109	Е	-	-
CI OH II	118	E	-	-
OH H H	643	E	-	-
CI CI CF3	264	E	E	E
CI SO2	563	E	-	<b>-</b>
CI CI CI	371	E	-	-
CI NOT	599	E	-	D

	N°		Target	
Compound		T-6	T-7	T-8
CI OH II	645	E	-	-
CI OH	497	E	<b>.</b>	C
CI HI O	644	E	-	-
CH CO	646	Е	-	E
CI CF3	649	В		D _.
DH THE COLUMN TO	498	E	-	-

	N°		Target	Target		
Compound		T-6	T-7	T-8		
CI H H	499	Е	-	-		
CI OH S	343	E	<b>-</b>	-		
CI S CI	441	Е	-	-		
OH IS S	385	E	-	-		
ÖH H S	399	E	-	C·		
HO CI	1296	E	E	E		
HO CI	1273	E	Е	Е		

	N°		•	
Compound		Т-6	T-7	T-8
CI HO CI	703	E	D	E
CI HO CI .	710	E	-	-
HO CI	716	E	-	· <b>-</b>

As may be taken from table 3 none of the tested compound is a strong inhibitor of any of the key proteases tested.

### Example 37: Cytotoxic effects on tumor cell lines

In order to show that the compounds according to the present invention are actually useful in the treatment of tumors, the cytotoxic effects of some of said compounds on tumor cell lines were determined.

For this cytotoxic evaluation of the compounds the commercial available WST-1 assay (Roche) was used according to the manufacturer's instructions. The assay is based on the cleavage of the tetrazolium salt WST-1 by mitochondrial dehydrogenases found in viable cells. In general compounds were added to cells cultured in 96-well plates at  $37^{\circ}$ C. After 48 h of incubation 10  $\mu$ l of WST-1 solution was added. The formazan dye was analyzed with an ELISA plate reader at (450 vs. 620) nm.

The following tumor cell lines were used in this assay:

CL-1: human acute myeloid leukemia, HL-60

CL-2: human cervix carcinoma, HeLa

CL-3: human prostate carcinoma, PC-3

CL-4: human colon adenocarcinoma, Caco-2

CL-5: human breast adenocarcinoma, MCF-7

In order to cluster the efficacy of the various compounds the following classes in terms of EC50 were defined.

A: EC50 < 10  $\mu$ M

B:  $10 \mu M < EC50 < 50 \mu M$ 

C:  $50 \mu M < EC50 < 100 \mu M$ 

D:  $100 \mu M < EC50 < 200 \mu M$ 

E: EC50 > 200  $\mu$ M

Table 4 Cytotoxic effects on tumor cell lines

	N°	Target					
Compound		CL-1	CL-2	CL-3	CL-4	CL-5	
CI NOH NO	102	A	A	<b>A</b>	A	. A	
CF3	261	A	В	В	В	В	
CI CF3	264	A	A	A	A	A	

	N°	Target						
Compound		CL-1	CL-2	CL-3	CL-4	CL-5		
CI S S	109	В	A	В	-	A		
CI S	254	В	В	В	-	В		
CI OH THE THE THE THE THE THE THE THE THE TH	30	A	-	-	A	-		
CI HN S CF3	221	В	-	-	-	В		
OH IN IN	6	В	-	-	-	A		
CI N N N N	54	В	-		-	A		
F OH	150	В	<u>.</u>	-	-	A		

	N°		Target						
Compound		CL-1	CL-2	CL-3	CL-4	CL-5			
E T Z W	639	A	-	-	<del>-</del>	<b>B</b>			
OH H H	640	В	· -	- -	-	<b>B</b>			
CI N	653	A	-	-	-	В			
CI S S	629	A	A	<b>A</b> .	-	<b>A</b>			
CI OH N	645	A	A	A	-	A			

	N°			Target		
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
OH H S	329 .	В	В	В	· -	В
CI OMB	493	В	<b>A</b>	<b>A</b>	-	-
CI CI	484	В	A	A	-	-
CI CI	483	ı	В	В	-	1
F CI	399	A	A	A.	-	A
OH HN S	654	-	В	-	-	Α

				Target	Target			
Compound		CL-1	CL-2	CL-3	CL-4	CL-5		
F OH II S	357	<b>A</b>	A	A	-	-		
OH OH S	413	В	A	В	-	-		
F OH H S	402	В	В	В	-	-		
CI CI CI	332	B _.	В	В	-	-		
OH H S	630	В	A	<b>A</b>	-	-		
F OH H S CI	403	В	A	A	-	-		

	N°	Target				
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
DH N N N N N N N N N N N N N N N N N N N	631	A	-	В	-	. <del>-</del>
OH HN O CI	632	A	- -	В	- -	-
CI HN CI	633	A	-	A	-	-
OH N OH CI	673	-	-	-	-	A

	N°			Target		
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
CI HN S CI	652	<b>A</b>	-	<b>A</b>	-	<del>-</del> -
HO CI	1273	В	· C	В	В	-
CI HO CI	703	В	В	В	В	-
HO CI	1296	С	-	-	-	-
CI HO CI	1297	С	-	<b>-</b>	<b>-</b>	-
HO S CI	1044	В	В	В	-	-

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As may be taken from table 4 all of the tested compounds are highly efficient in exhibiting a cytotoxic effect on at least one of the various tumor cell lines tested. Of particular relevance are compounds 102, 264, 357, 399, 629, 633, 645, 652, 673, 703, 1044, 1273.

# Example 38: FACS measurements and TUNEL assay

In order to show that the compounds according to the present invention are actually useful for inducing apoptosis in tumor cells, FACS measurements and TUNEL assay were performed. Enari M. Sakahira H. Yokoyama H. Okawa K. Iwamatsu A. Nagata S. A caspase-activated DNase that degrades DNA during apoptosis, and its inhibitor ICAD [erratum appears in Nature 1998 May 28;393(6683):396.]. Nature. 391:43-50, 1998

Darzynkiewicz Z. Juan G. Li X. Gorczyca W. Murakami T. Traganos F. Cytometry in cell necrobiology: analysis of apoptosis and accidental cell death (necrosis). Cytometry. 27:1-20, 1997

Apoptotic HL-60 cells were detected by FACS analysis of FITC-dUTP-labelled DNA breaks using the Apo-Direct kit (BD-Pharmingen) according to the manufacturer's protocol.

As may be taken from Fig. 2 compounds 102 and 264 induce apoptosis in tumor cells.

### Example 39: Cyclin D1 down regulation

In order to show that the compounds according to the present invention are actually acting the expected way and induces cyclin D1 down regulation, cyclin D1 marker analysis were performed

MCF-7 (5×10⁵ cells/well) and HeLa cells (1.5×10⁵ cells/well) were seeded in 6-well plates and incubated at 37°C over night. Compounds or DMSO (final solvent concentration 0.1%) were added to the cells and incubated for different times as indicated. Subsequently, cells were lysed in RIPA buffer for 30 min on ice and centrifuged for 20 min at 4°C. After addition of electrophoresis sample buffer (4×) and 50 mM DTT to the supernatant, samples were

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boiled for 4 min at 95°C. Samples (equivalent to 2×10⁵ cells/well) were run on a 15% SDS gel followed by blotting onto PVDF membrane.

The membrane was blocked for 1 h in 10 mM Tris (pH 7.5), 100 mM NaCl, 0.1% Tween-20 and 5% non-fat dry milk (blocking buffer) and incubated for 1 h with mouse anti-hCyclin D1 monoclonal antibody (clone DCS-6, BD Biosciences) diluted to 1  $\mu$ g/ml in blocking buffer. Blots were washed 3 × 10 min with 10 mM Tris (pH 7.5), 100 mM NaCl, 0.1% Tween-20 (washing buffer) and incubated with 0.7  $\mu$ g/ml peroxidase-conjugated sheep anti-mouse IgG (Sigma) in blocking buffer for 1 h. After washing 3 × 10 min with washing buffer, the plot was developed with the ECL+ detection kit (Amersham Biosciences).

Of particular relevance are compounds 30, 102, 264, 399, 629, 639, 657, 673.

## Example 40: DAPI staining

In order to show that the compounds according to the present invention are actually useful for inducing apoptosis in tumor cells, DAPI staining was performed.

Hela cells grown on poly-L-Lys-coated coverslips were fixed with 2% paraformaldehyde/MeOH.

Cellular DNA was stained with DAPI staining buffer (100 mM Tris (pH 7.4), 150 mM NaCl, 1 mM CaCl2, 0.5 mM MgCl2, 0.1% nonidet P-40, 1 µg/ml DAPI (Molecular Probes)). All the steps were performed at room temperature, and cells were washed two times with PBS after each step. Finally, cells were mounted in 80% glycerol/PBS.

As may be taken from Fig. 3 compounds 30, 102, 264 and 399 induce apoptosis in tumor cells.

The features of the present invention disclosed in the specification, the claims and/or the drawing may both separately and in any combination thereof be material for realizing the invention in various forms thereof.